

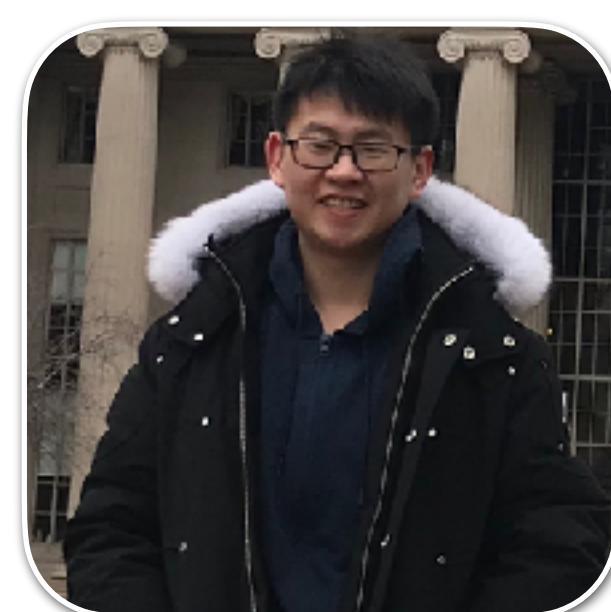
# Theoretically Grounded Framework for LLM Watermarking: A Distribution-Adaptive Approach

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Univ. of Florida



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Tongji Univ.



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Univ. of Ottawa



Prof. Yuheng Bu  
Univ. of Florida

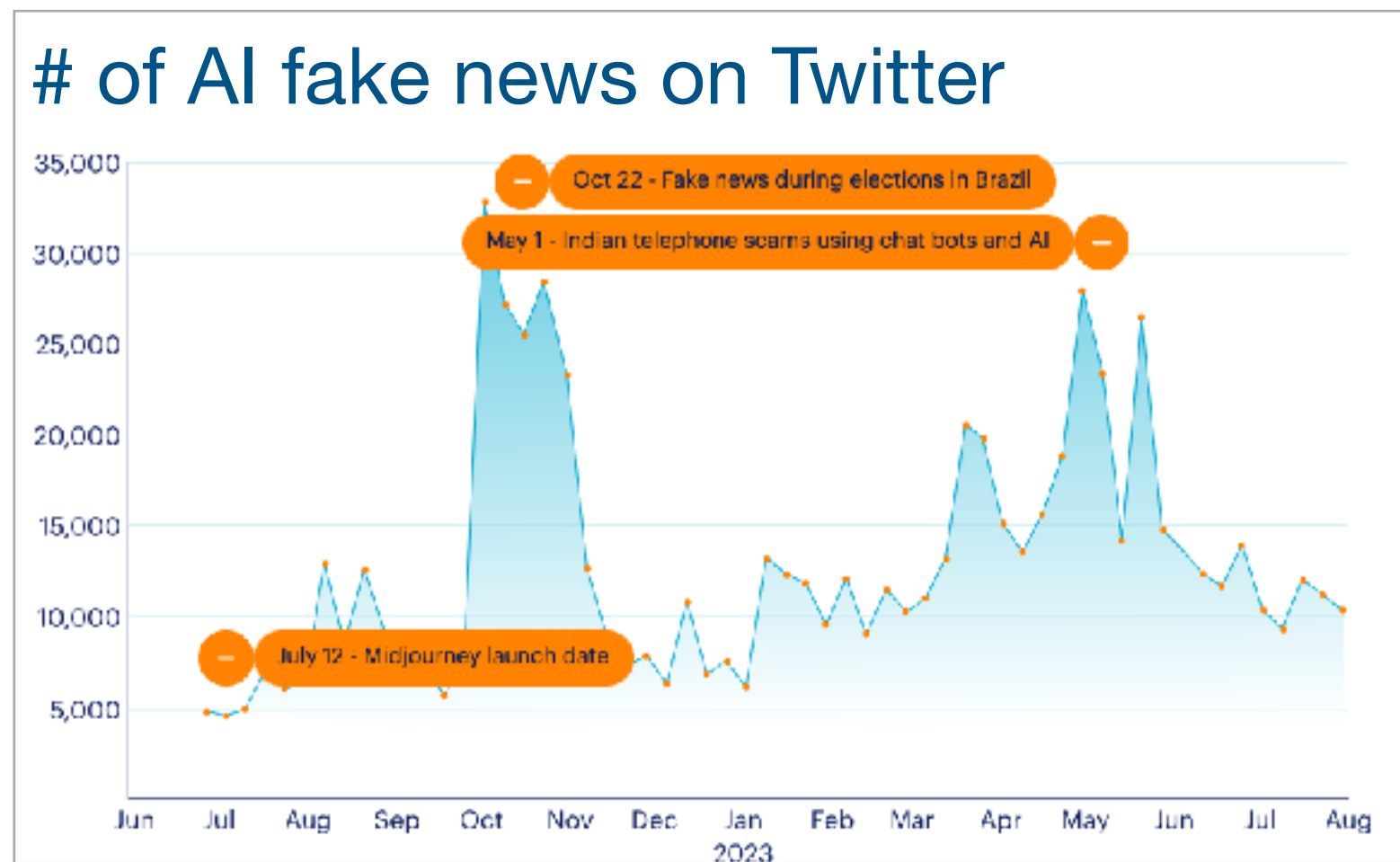
ITA 2025

# Challenges in AI Safety

Misuse of AI-generated content

# Challenges in AI Safety

## Misuse of AI-generated content



Fake news

# Challenges in AI Safety

## Misuse of AI-generated content



AI scams

# Challenges in AI Safety

## Misuse of AI-generated content



Plagiarism

# Challenges in AI Safety

Misuse of AI-generated content

Data Pollution



Plagiarism

# Challenges in AI Safety

## Misuse of AI-generated content



Plagiarism

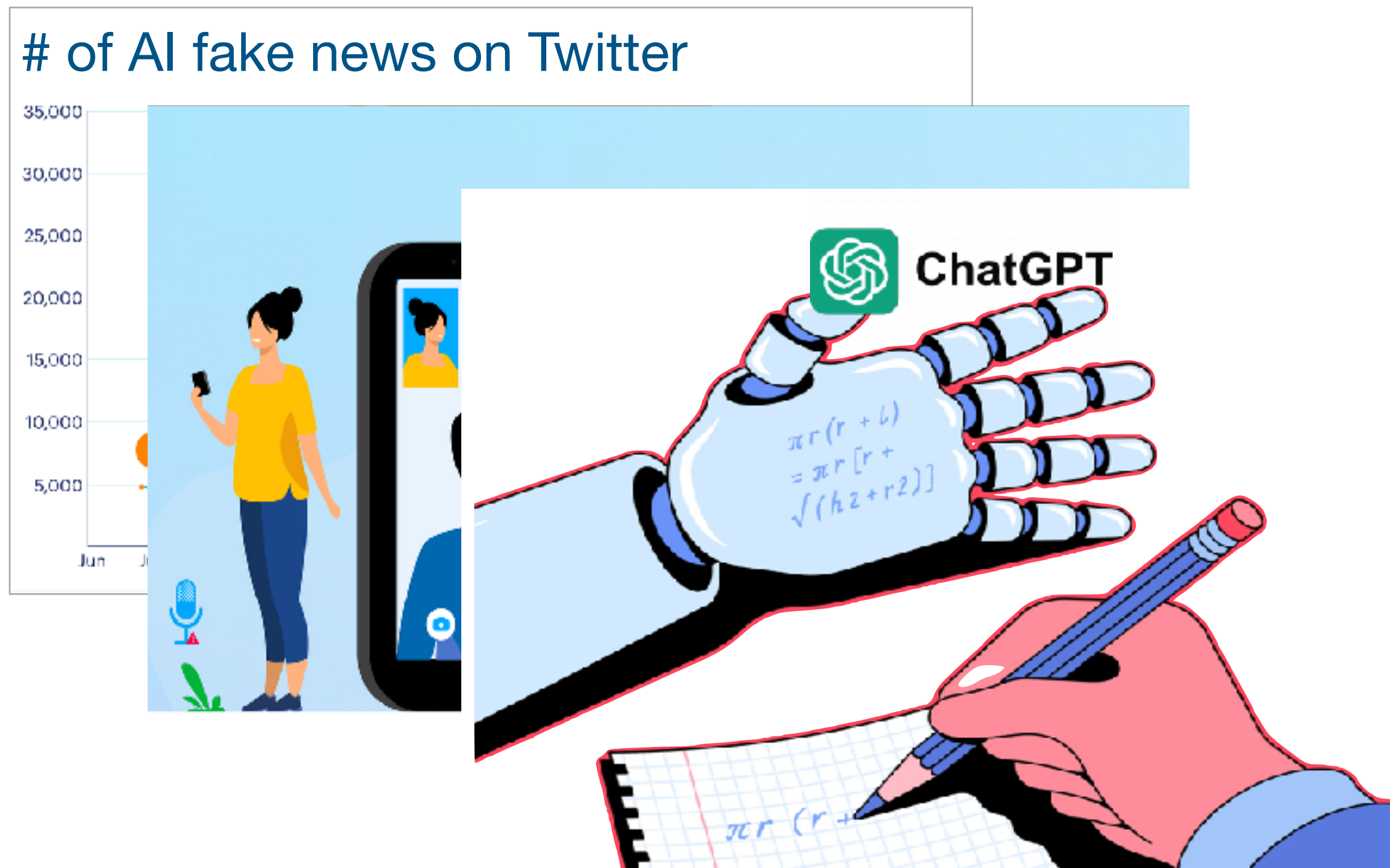
## Data Pollution

Tons of AI-generated data over the internet



# Challenges in AI Safety

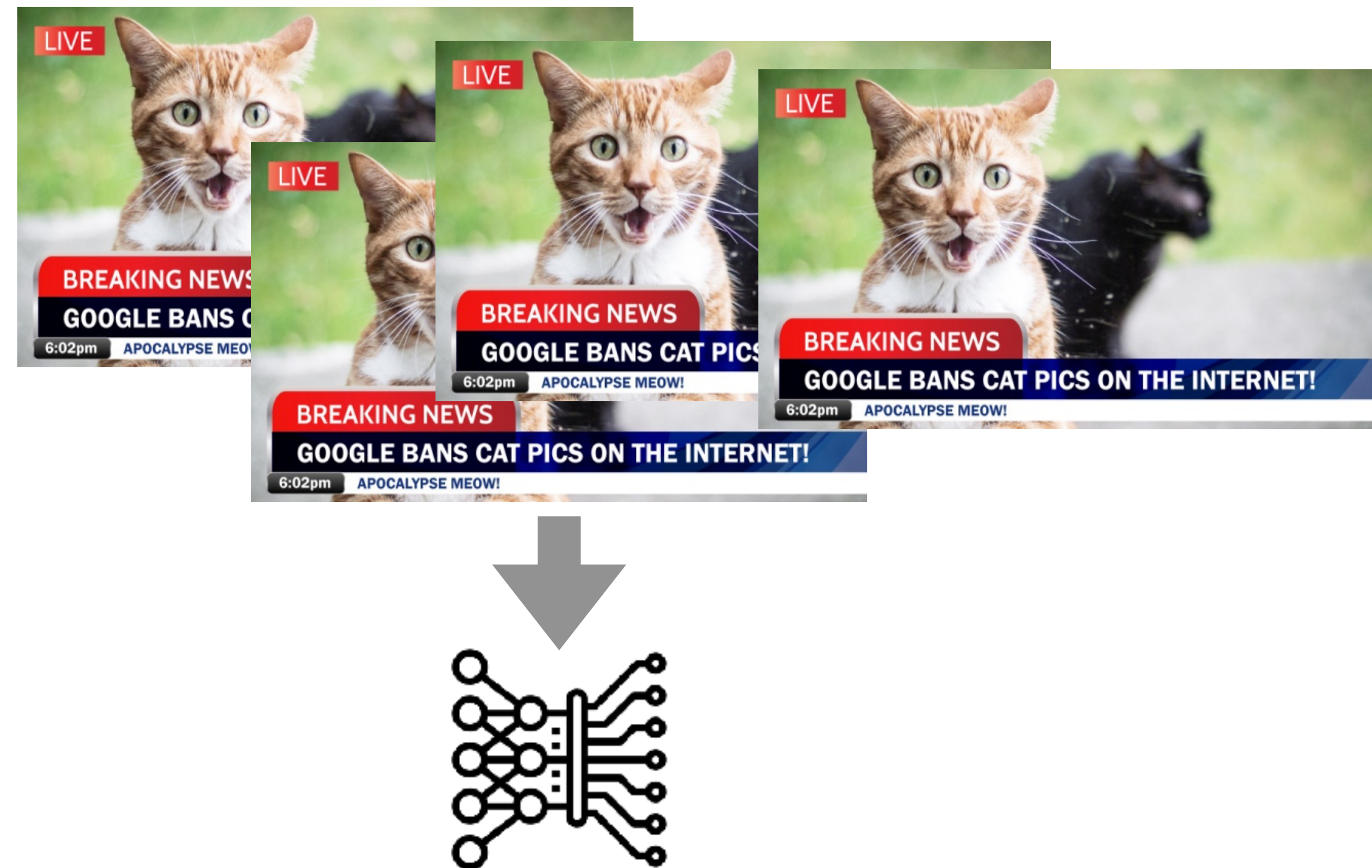
## Misuse of AI-generated content



Plagiarism

## Data Pollution

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# Challenges in AI Safety

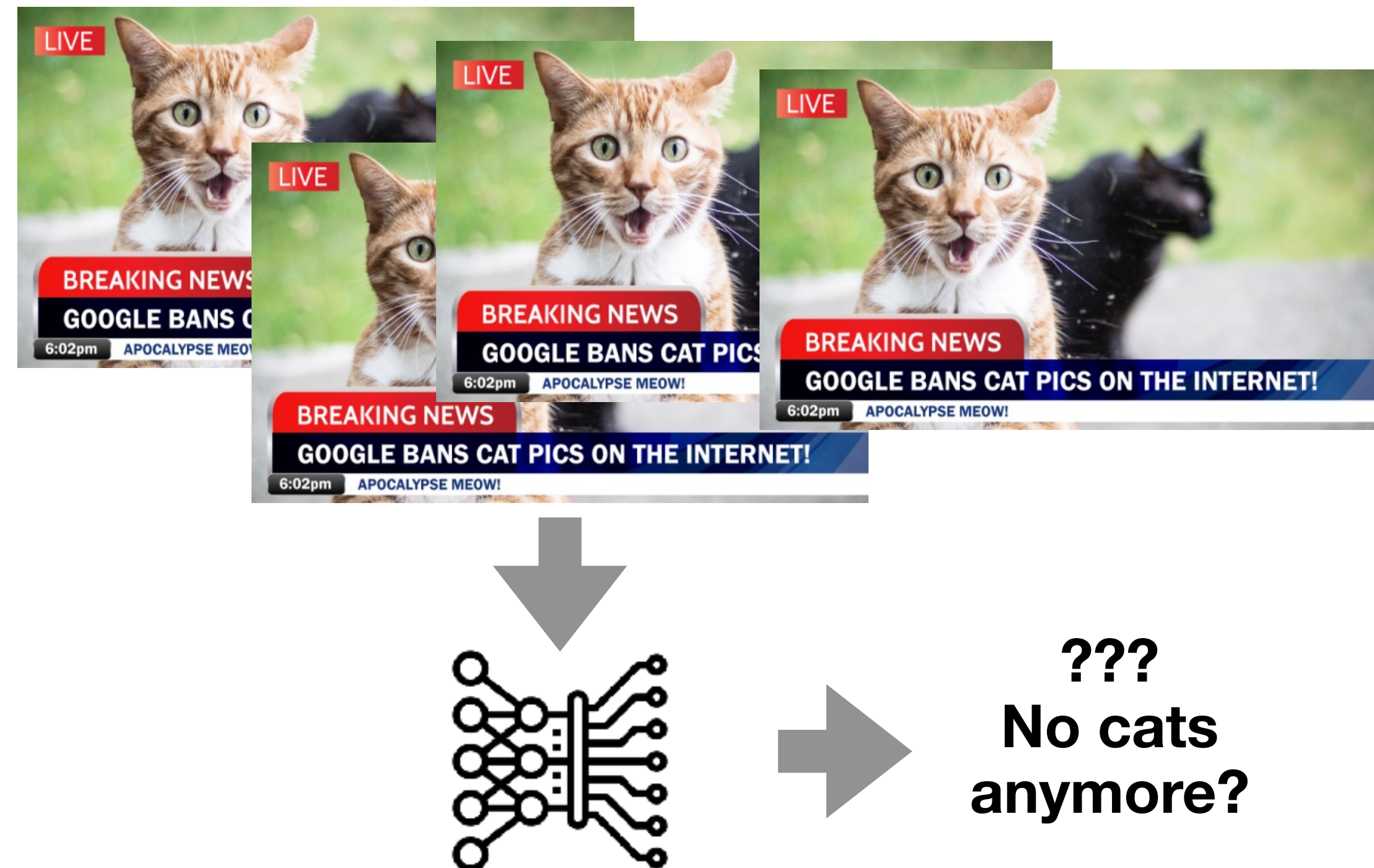
## Misuse of AI-generated content



Plagiarism

## Data Pollution

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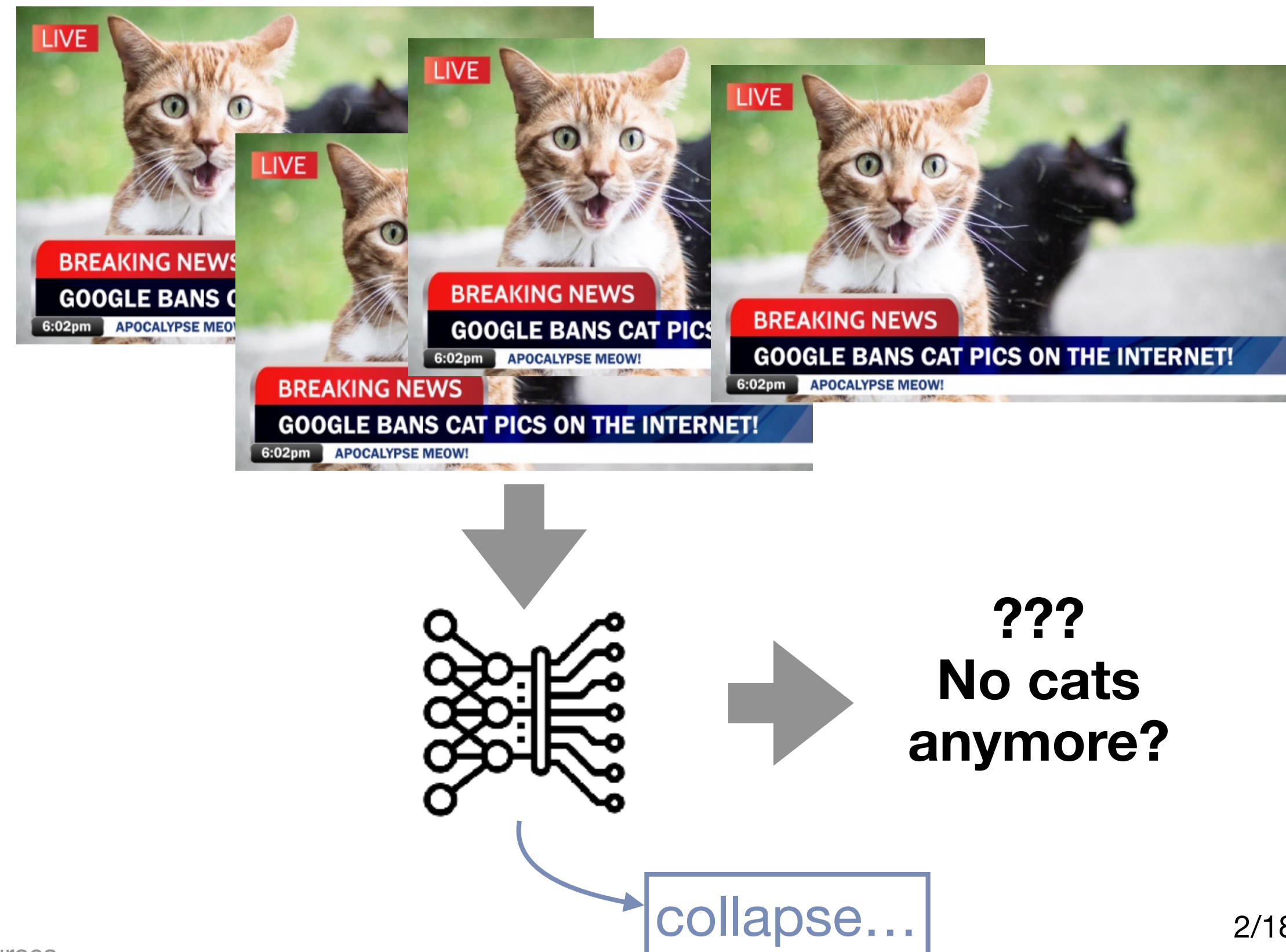
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## Misuse of AI-generated content



## Data Pollution

Tons of AI-generated data over the internet



# Challenges in AI Safety

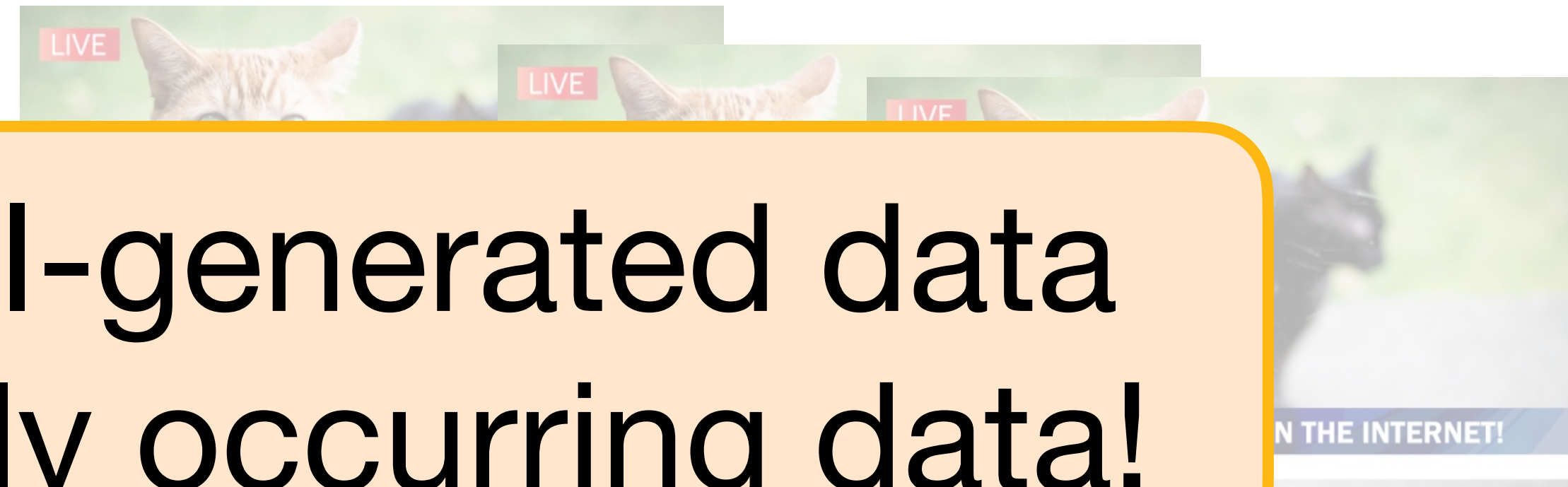
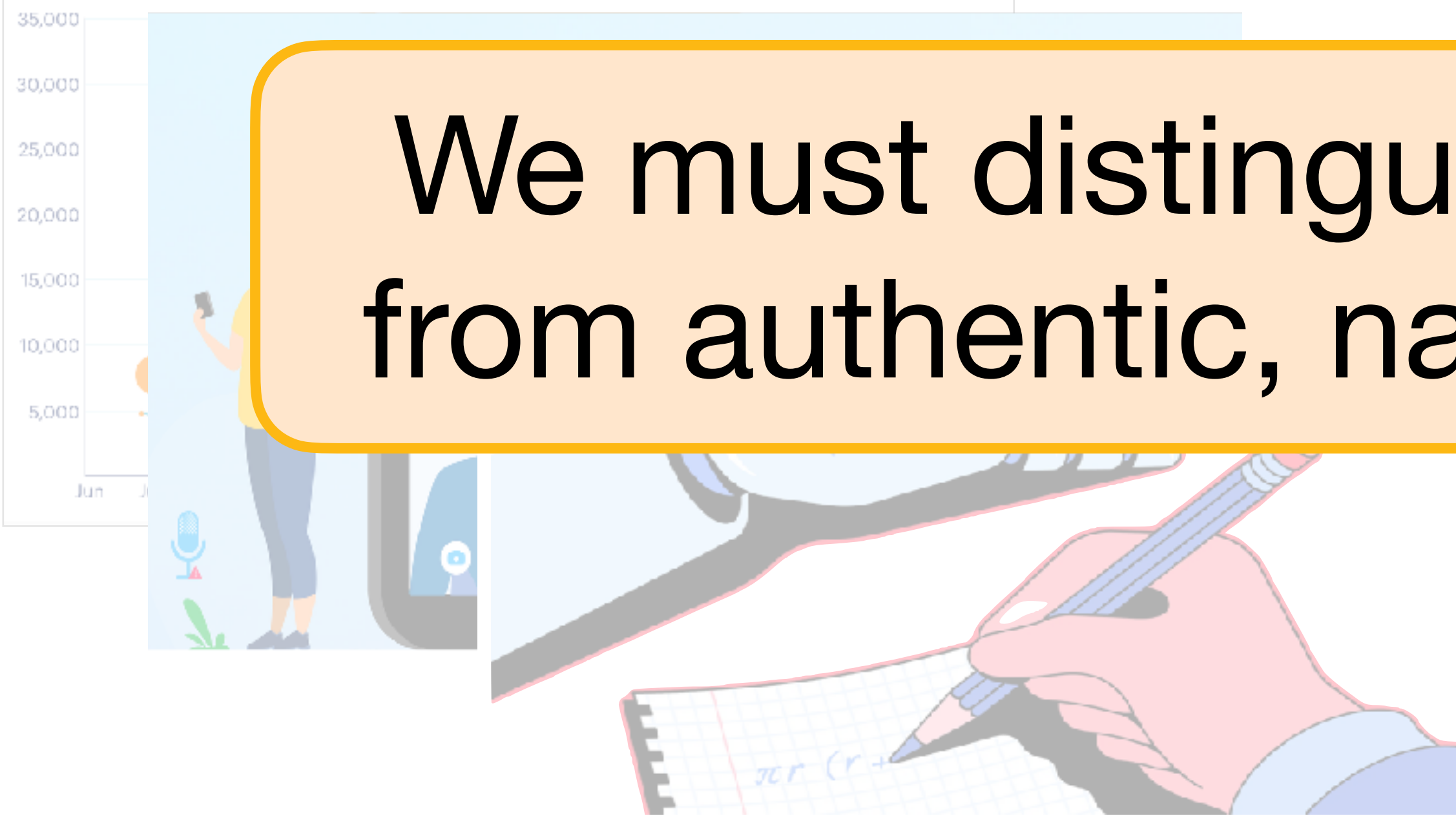
Misuse of AI-generated content

Data Pollution

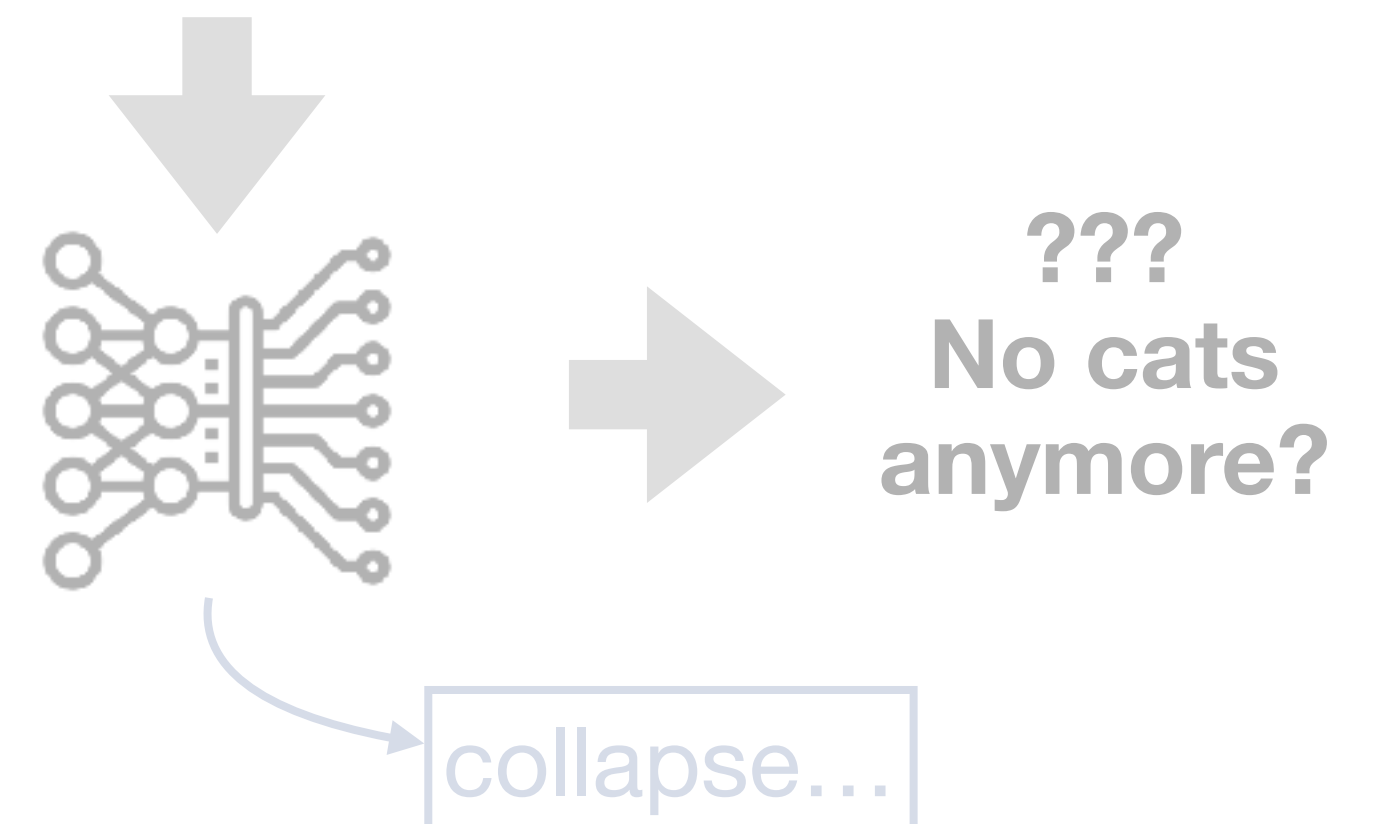
Tons of AI-generated data over the internet

**We must distinguish AI-generated data from authentic, naturally occurring data!**

# of AI fake news on Twitter



Plagiarism



# Identify AI-generated Text

Possible solutions?

# Identify AI-generated Text

## Possible solutions?

- By observation:

# Identify AI-generated Text

Possible solutions?

*“Here’s the revised version of your...”, “Best regards,[Your Name]”* :-D

# Identify AI-generated Text

## Possible solutions?

- Metadata ← easy to remove

**Metadata**

**File name:** Dataset  
**Author:** GPT  
**Location:** Ithaca  
**Created:** Jan 01, 2025

# Identify AI-generated Text

## Possible solutions?

- Giant database to store all AI-generated content <— storage? privacy?



# Identify AI-generated Text

## Possible solutions?

- Discriminator models:  **GPTZero**  **DetectGPT**  **Copyleaks**  **pangramlabs** ...

# Identify AI-generated Text

Possible solutions?

<— high prob of falsely alarming human-written text

# Identify AI-generated Text

Possible solutions?

- **Watermarking: inserting a signal into LLM predicted tokens**

# Identify AI-generated Text

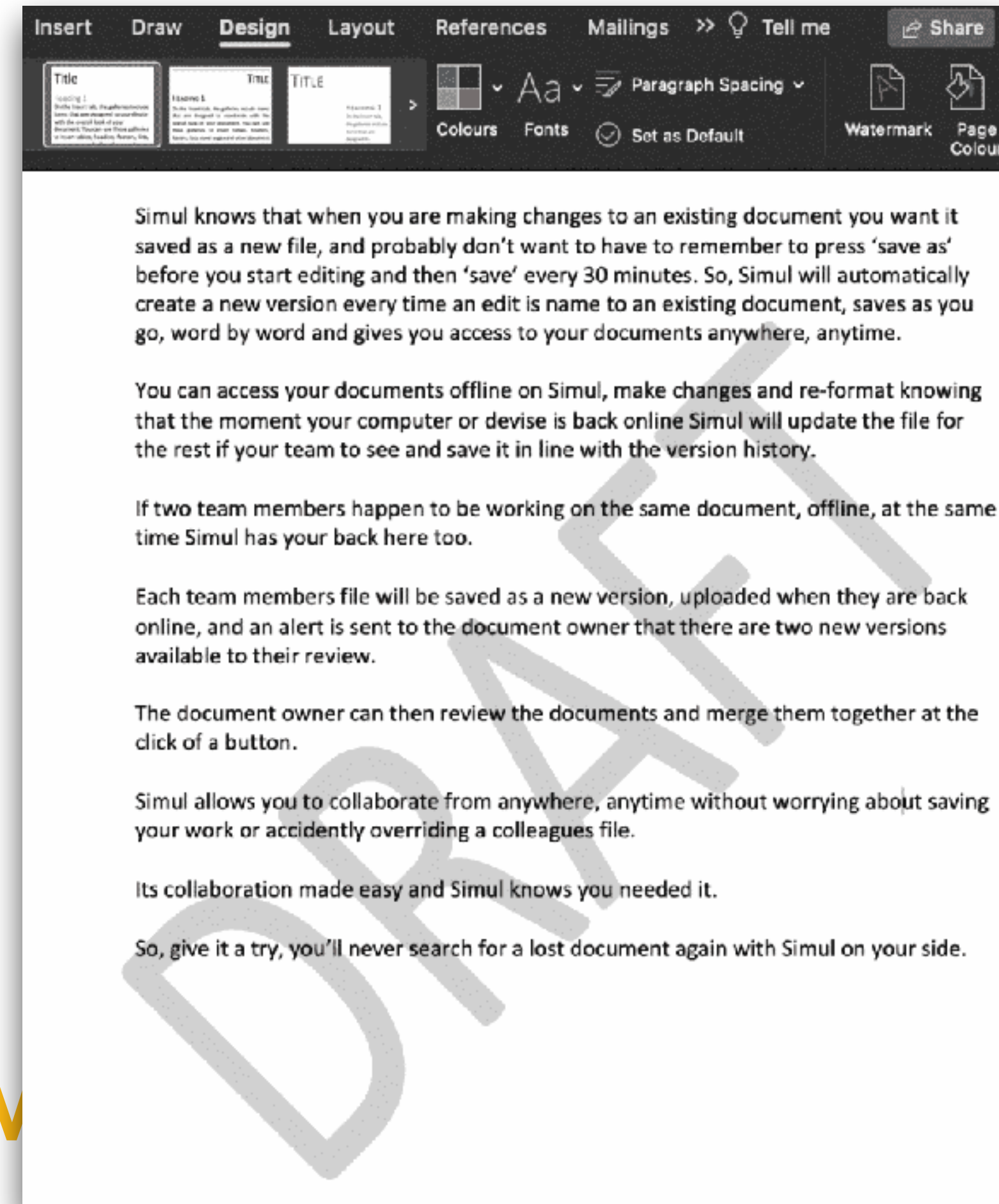
Possible solutions?



- **Watermarking: inserting a signal into LLM predicted tokens**

# Identify AI-generated Text

## Possible solutions?



- **Watermarking: inserting a signal into LLM**

# Identify AI-generated Text

Possible solutions?



- **Watermarking: inserting a signal into LLM predicted tokens**

# Identify AI-generated Text

Possible solutions?

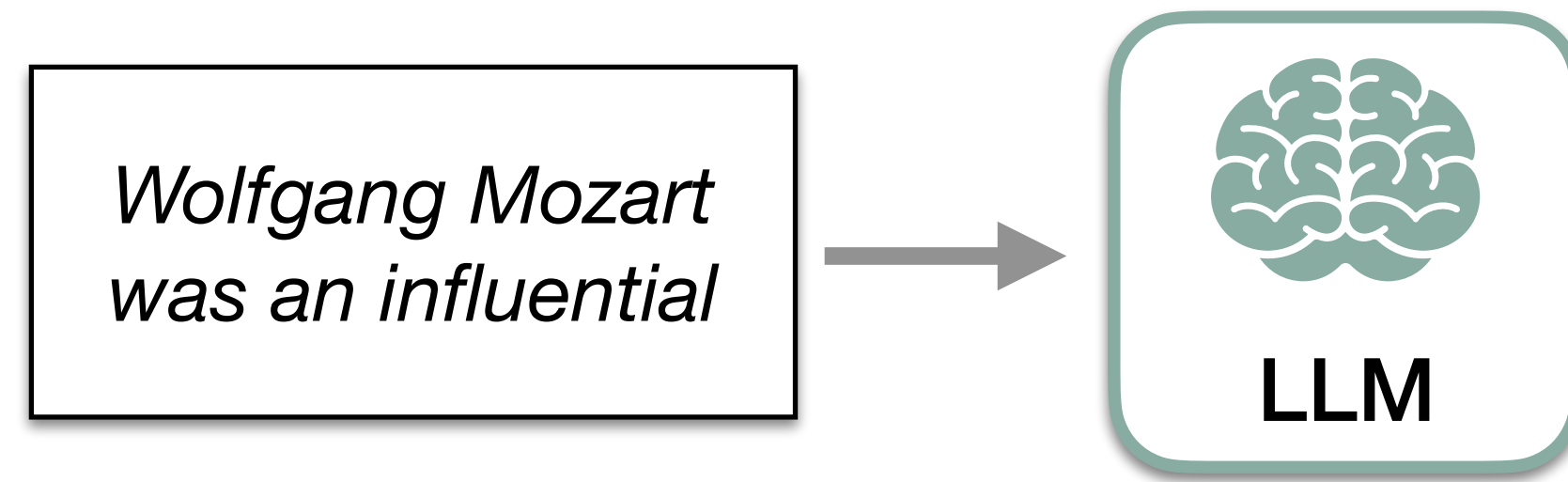
- **Watermarking: inserting a signal into LLM predicted tokens**



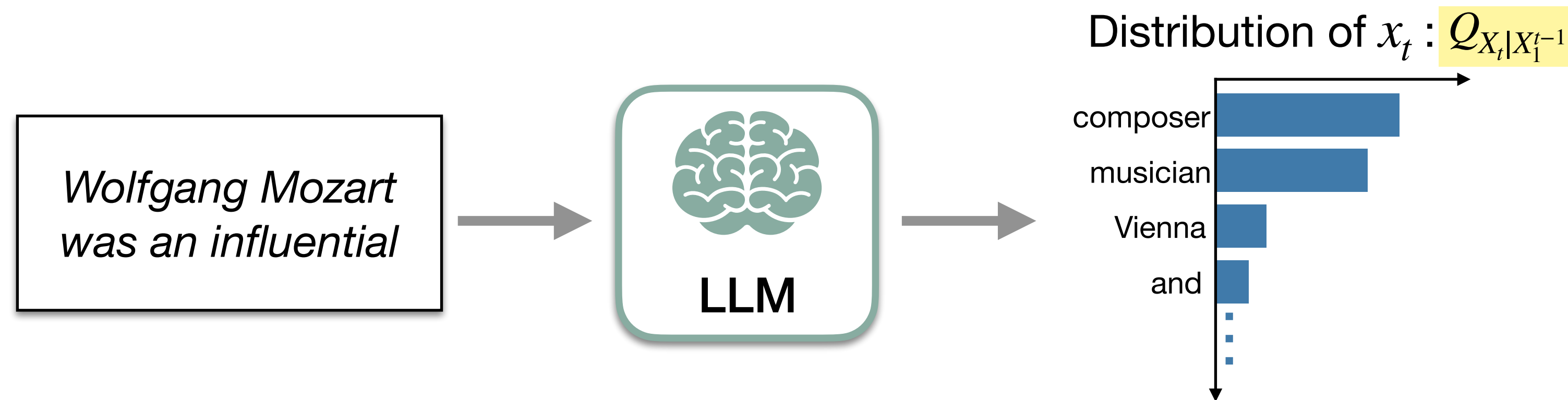
# A Framework for LLM Watermark Generation



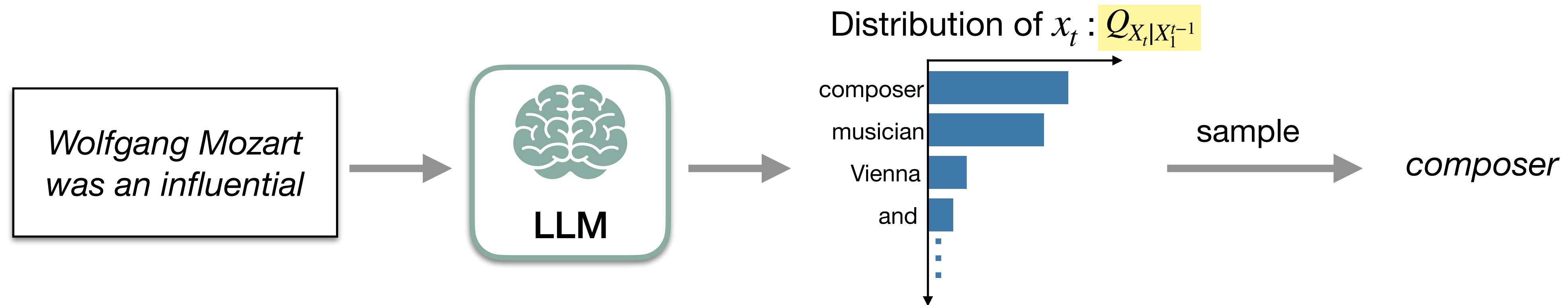
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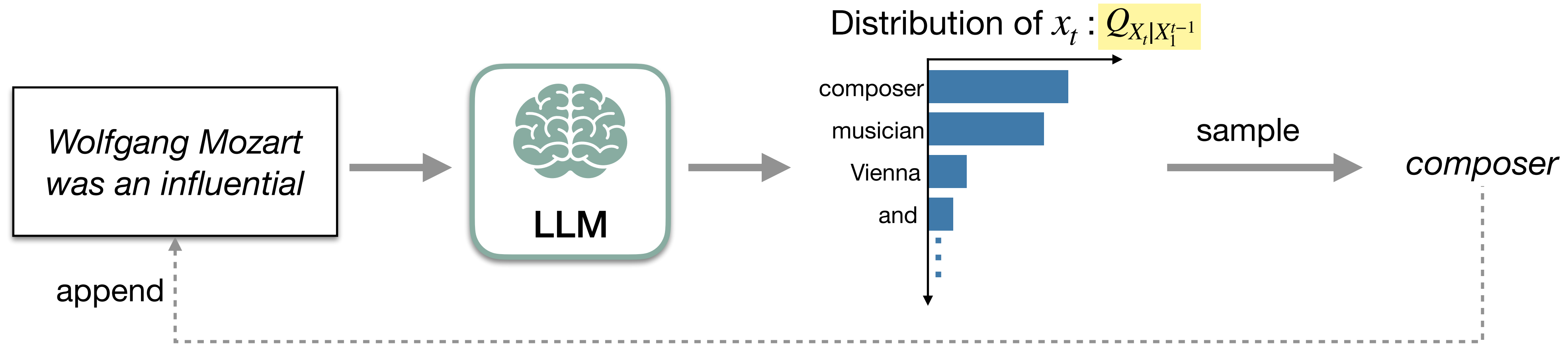
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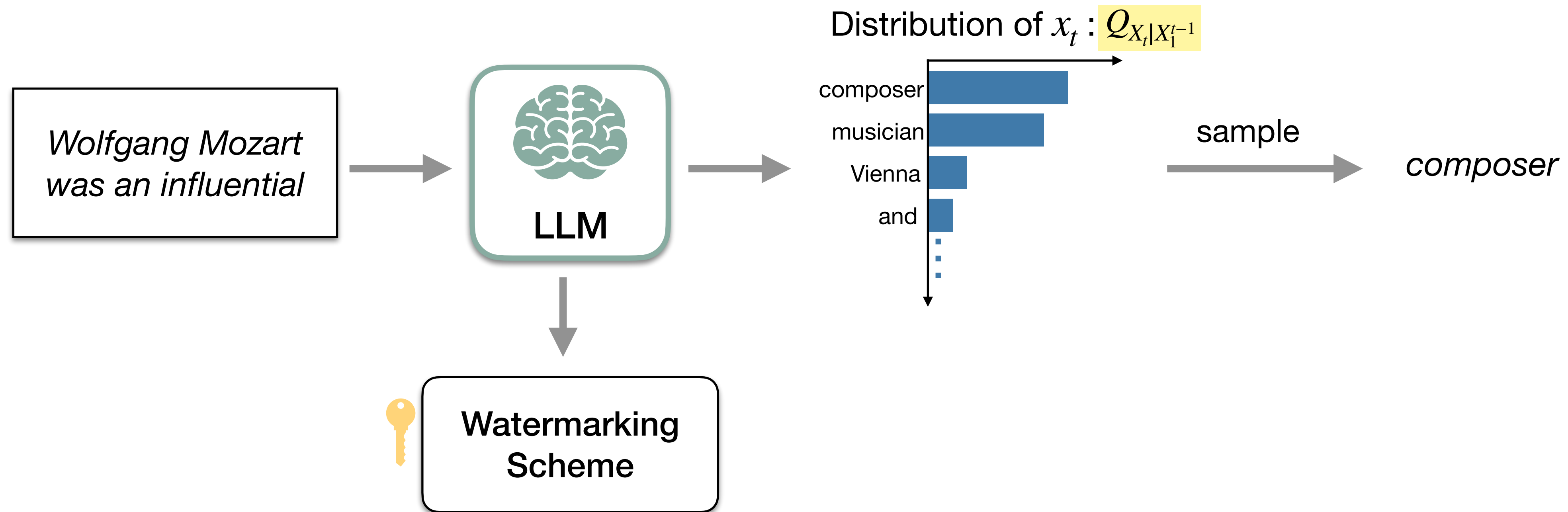
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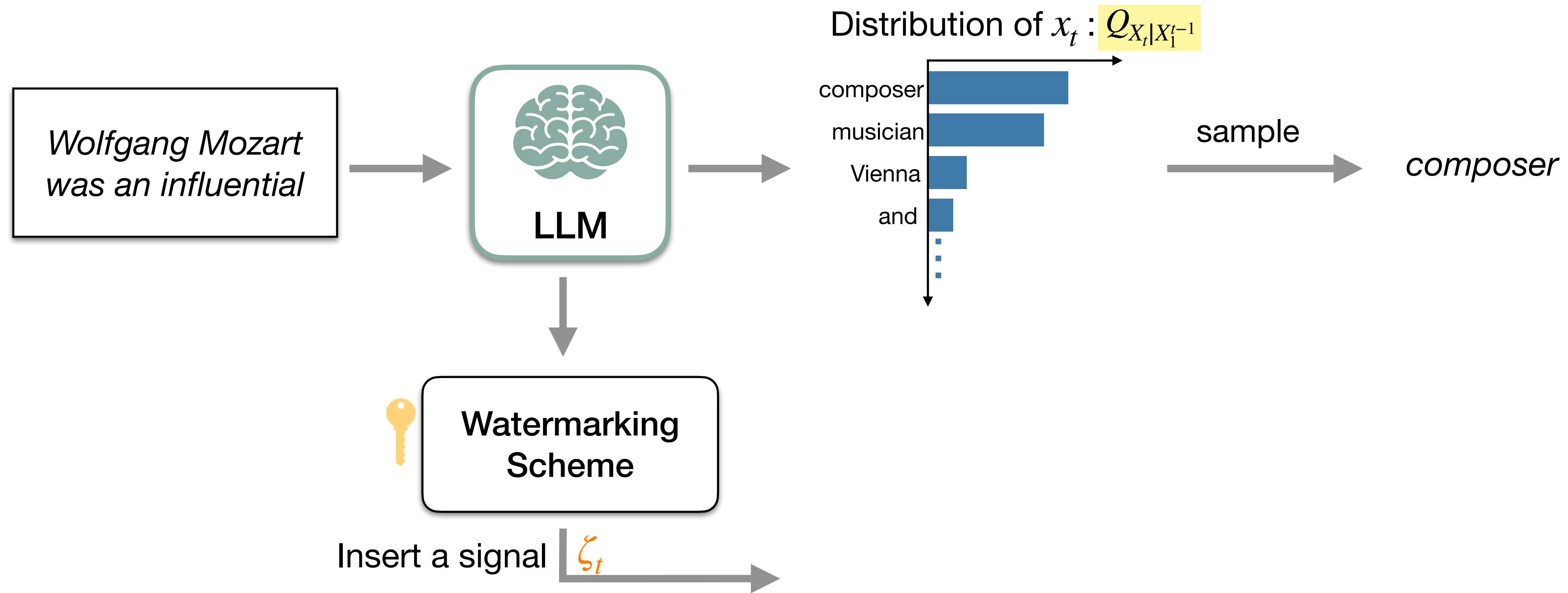
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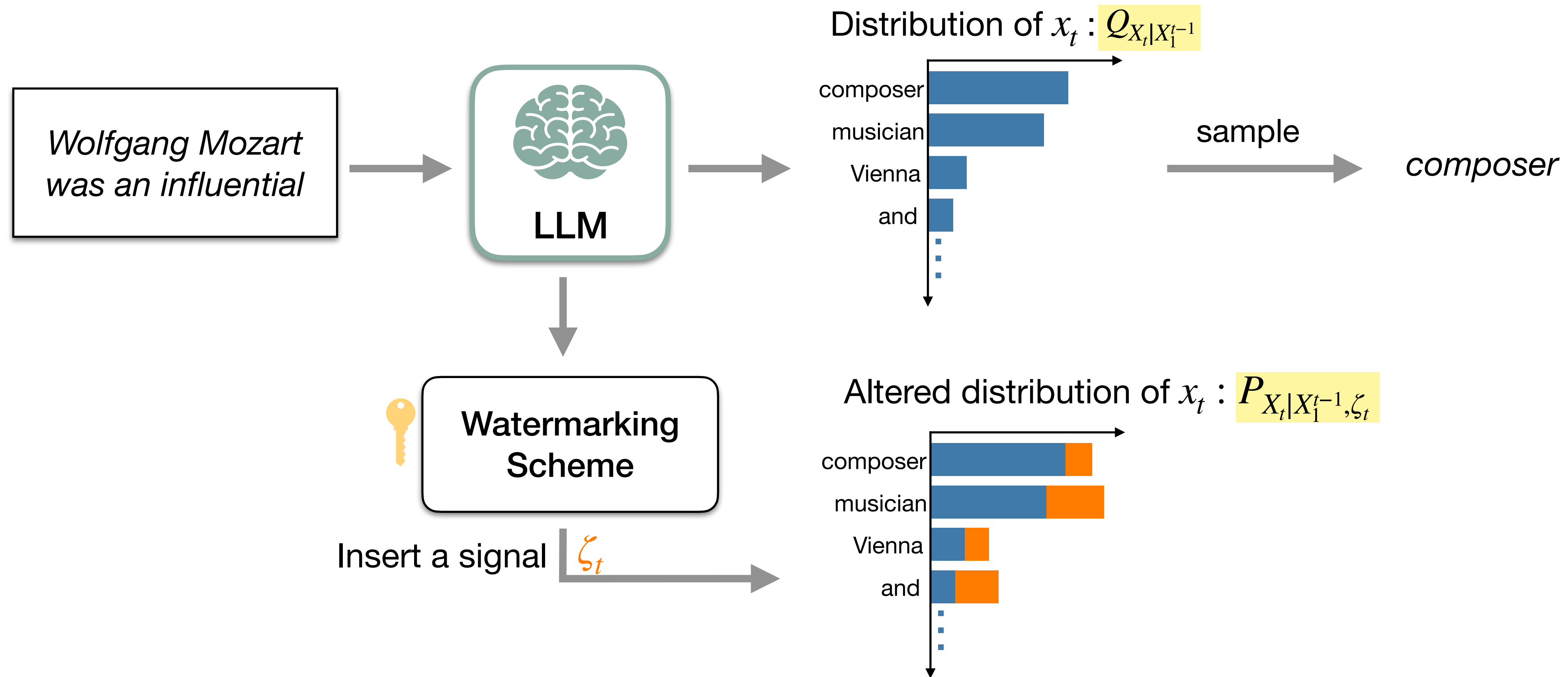
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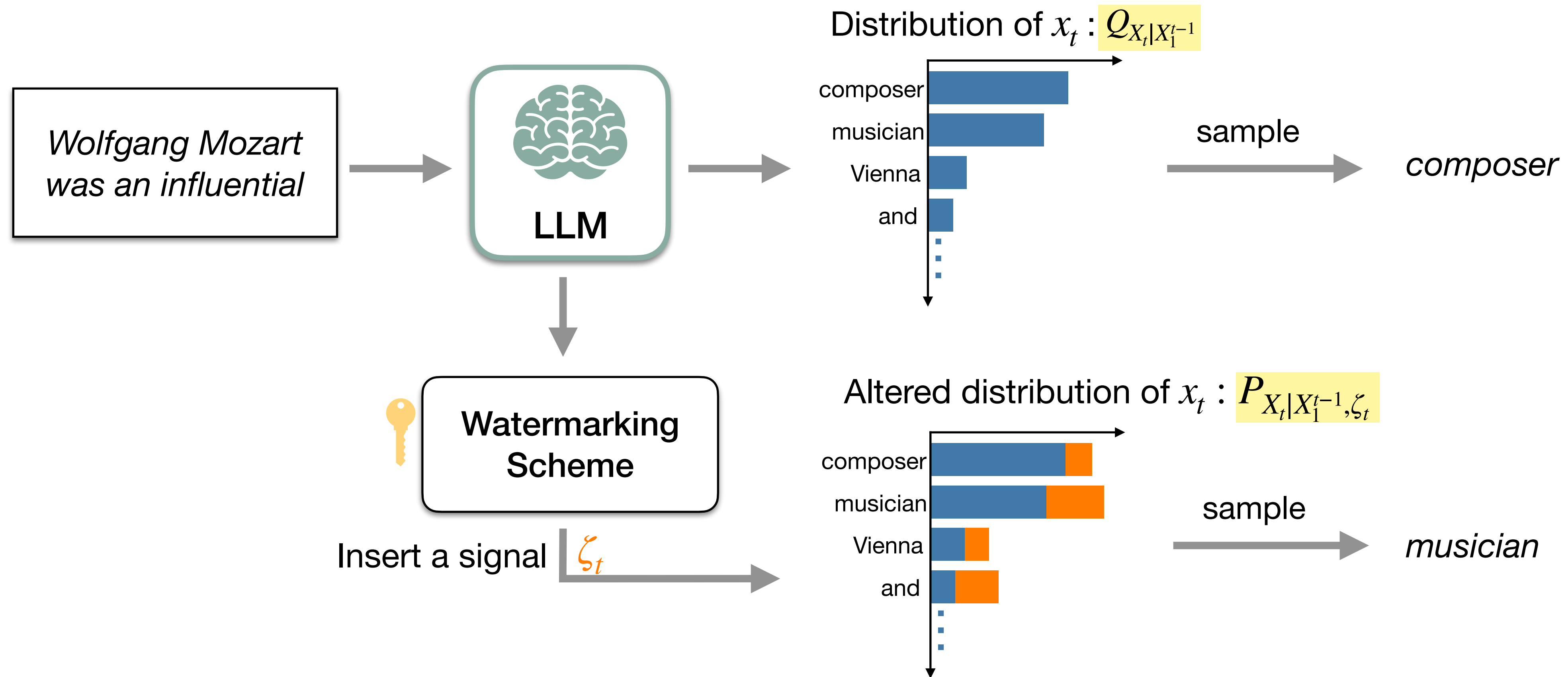
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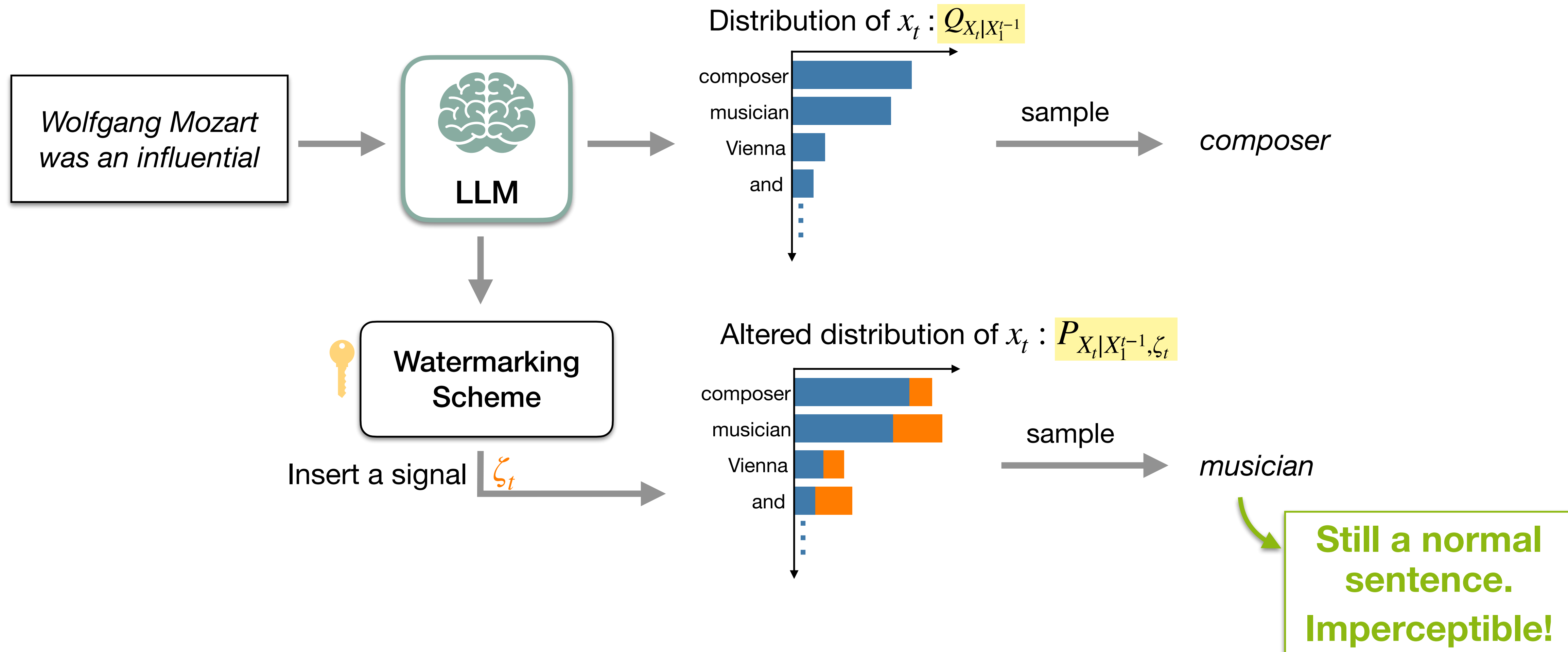


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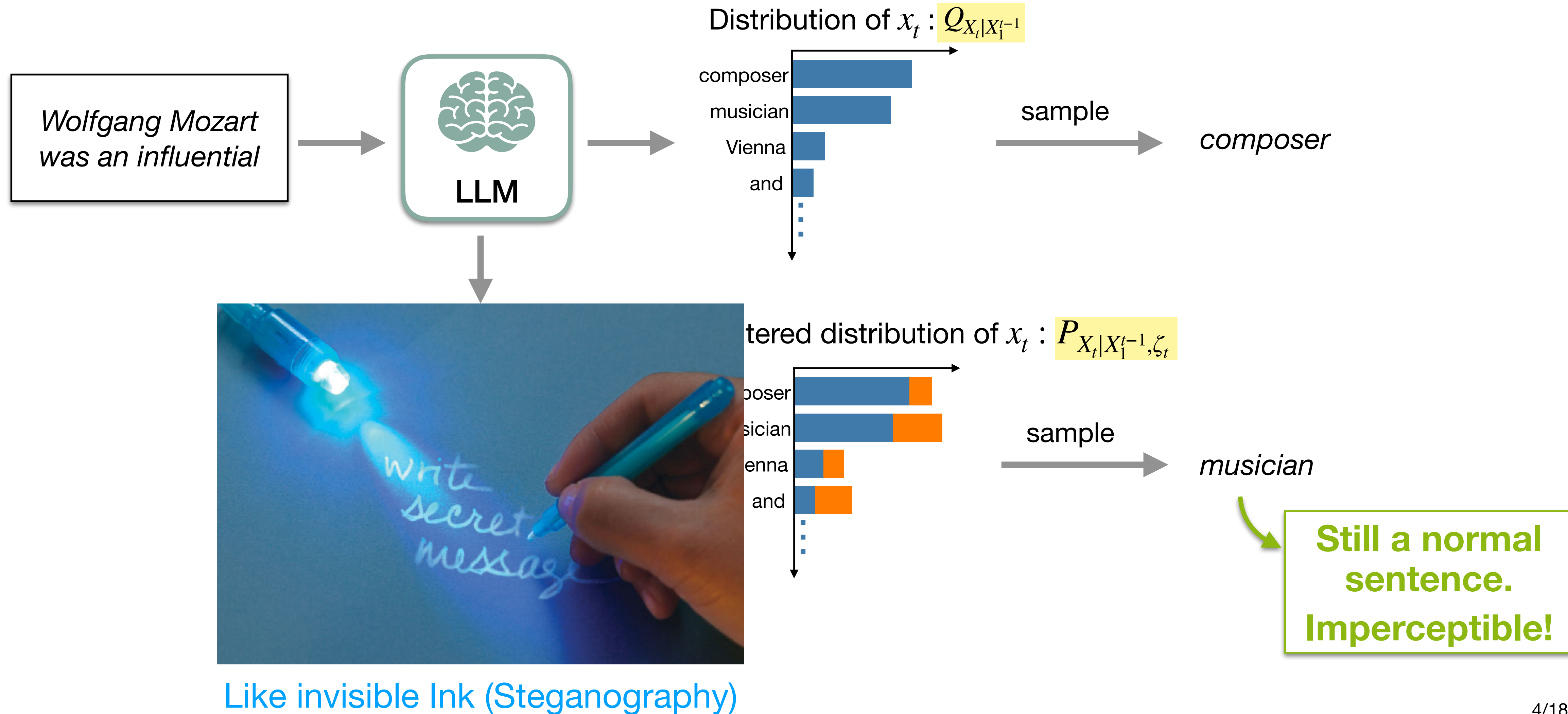




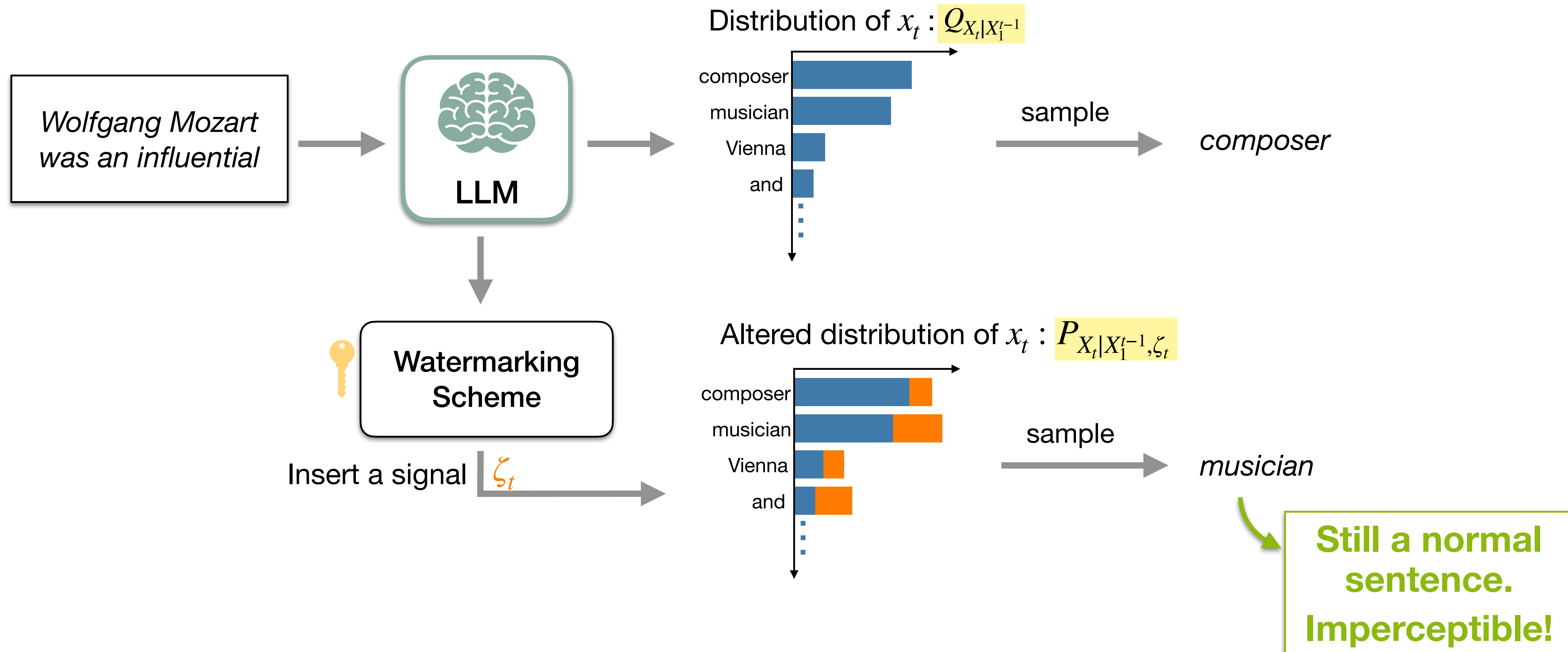
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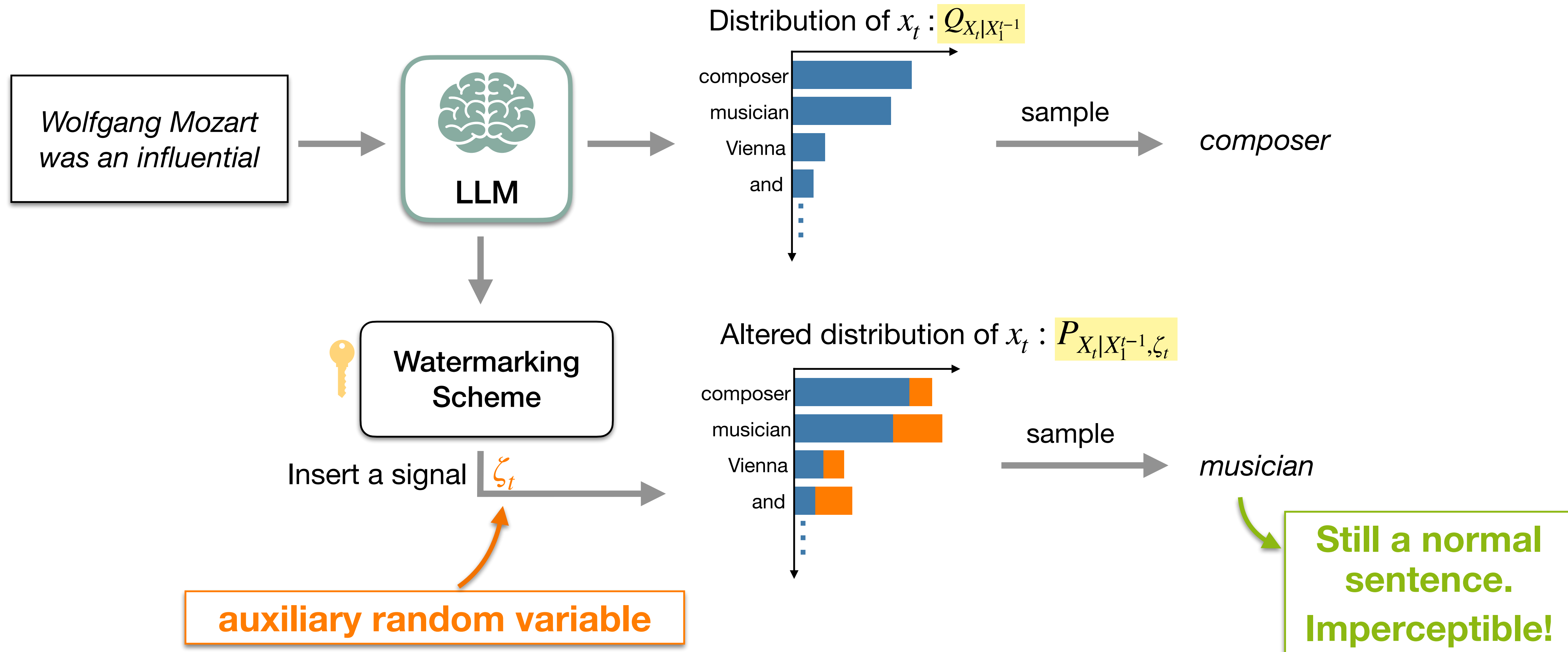
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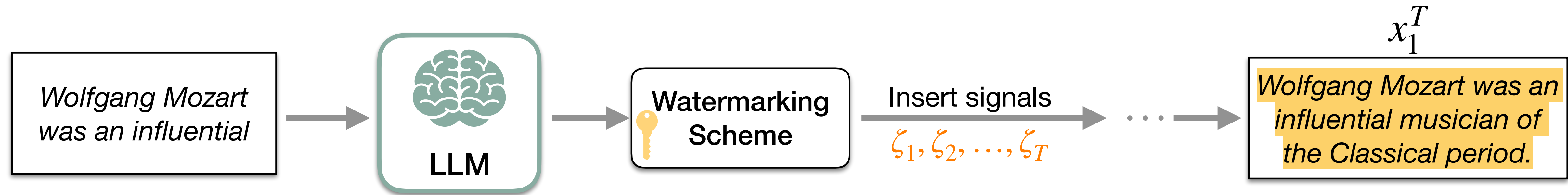
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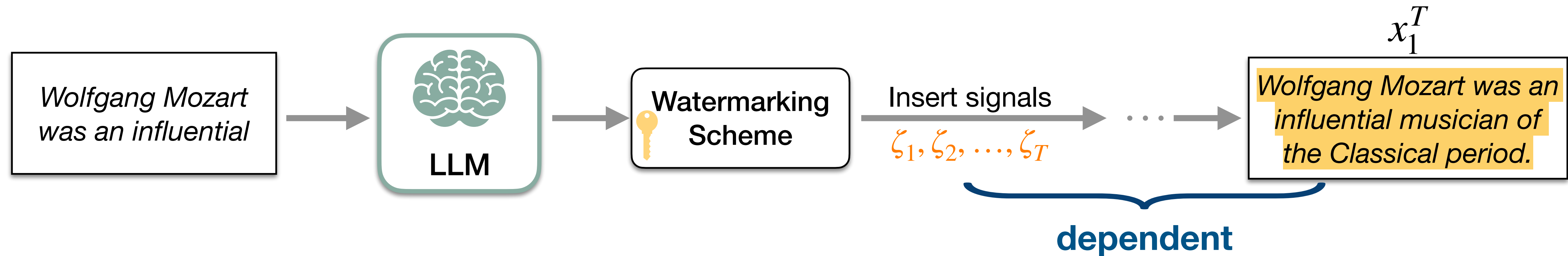
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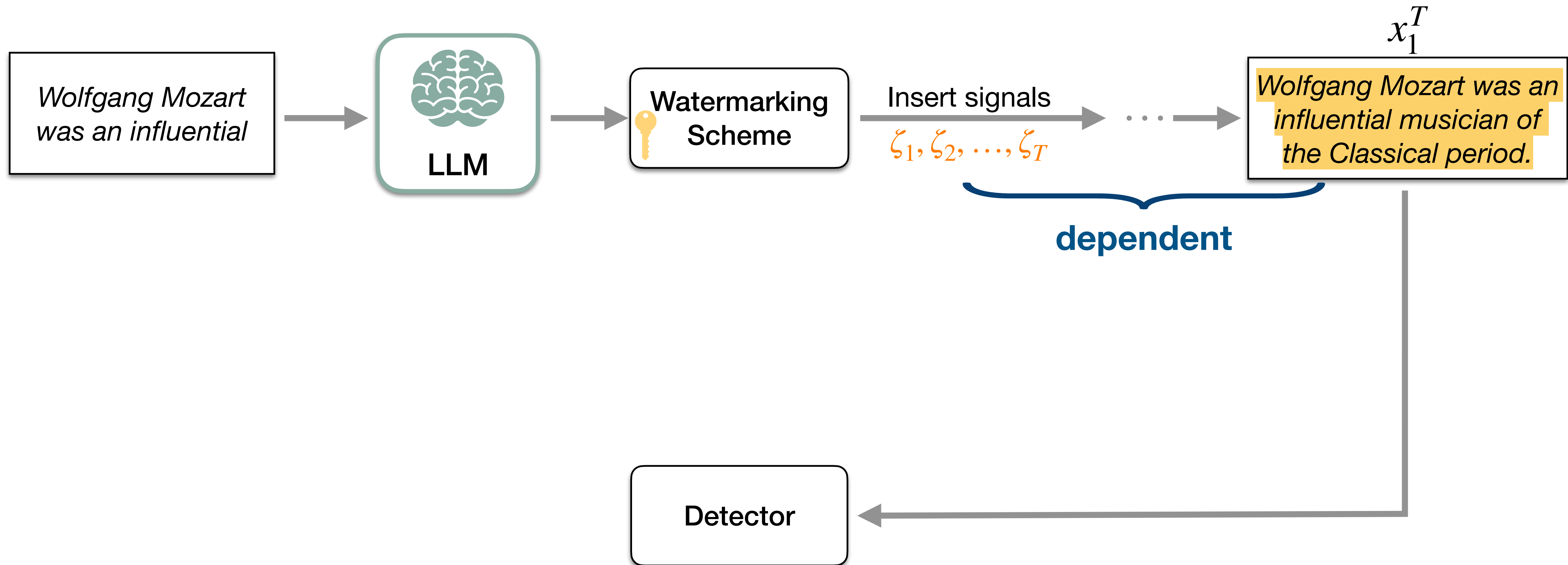
# Hypothesis Testing for LLM Watermark Detection



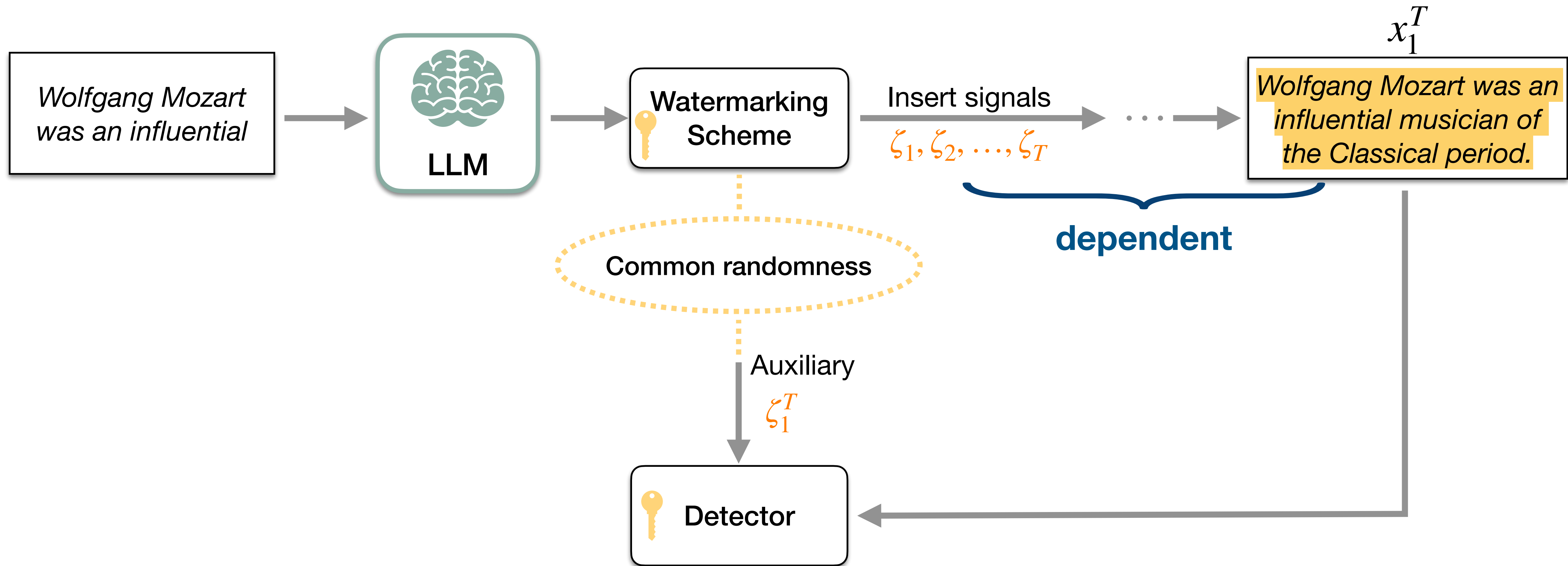
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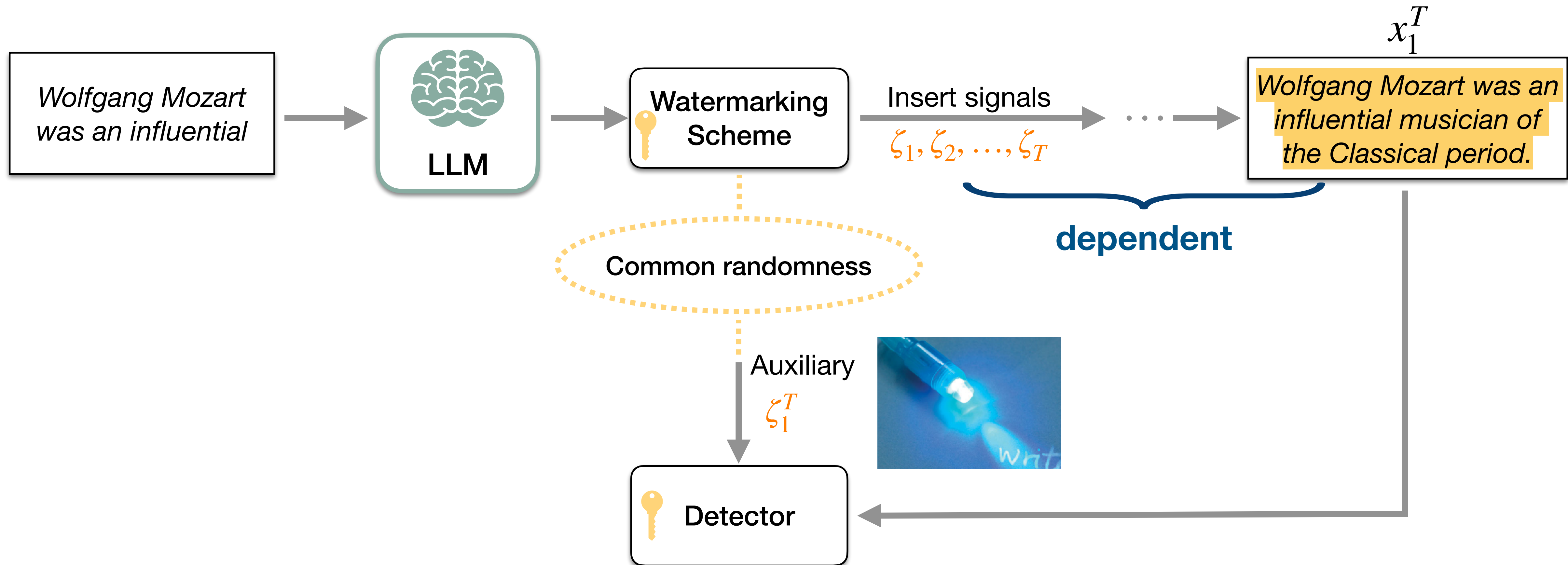


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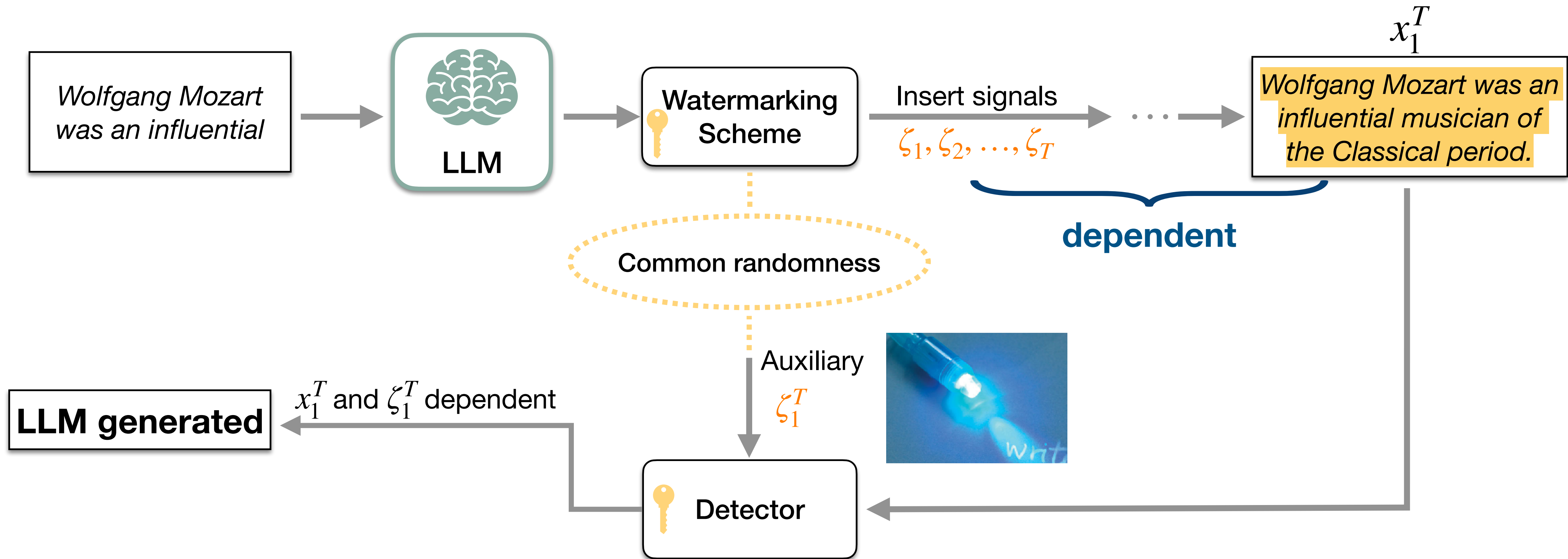




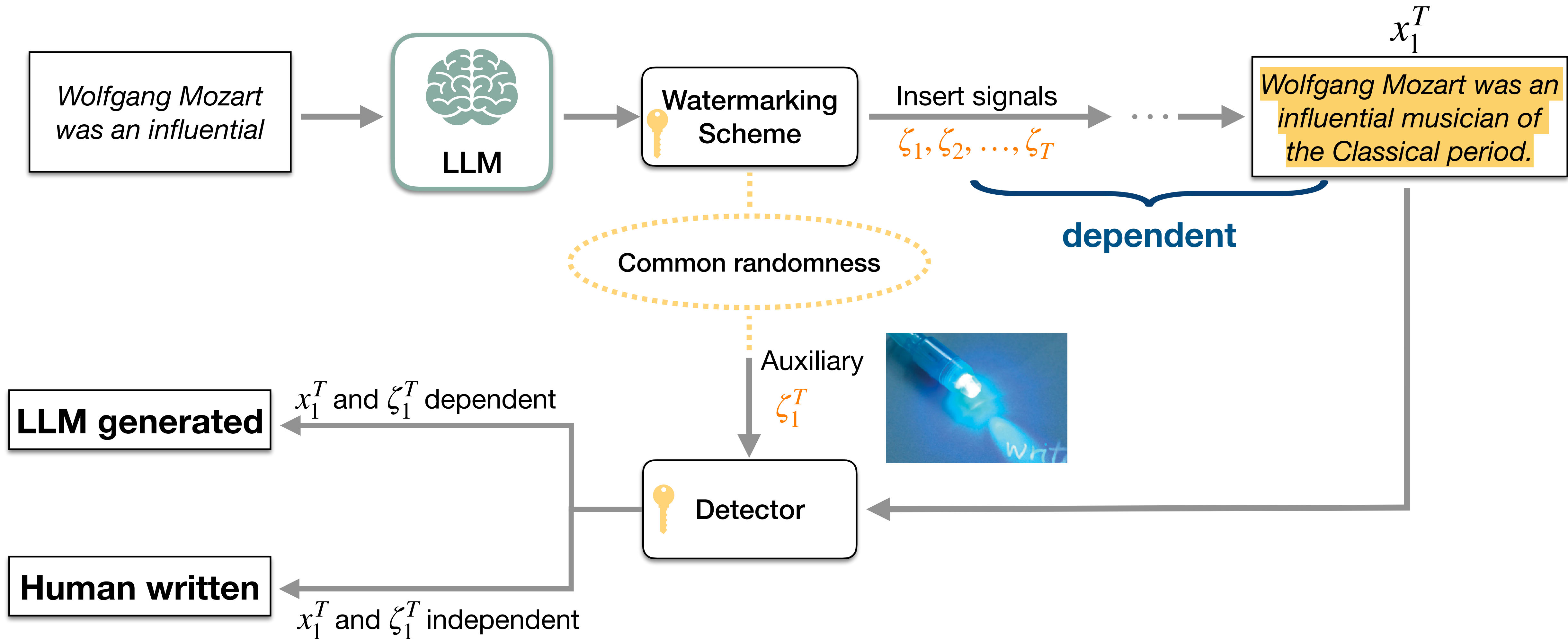
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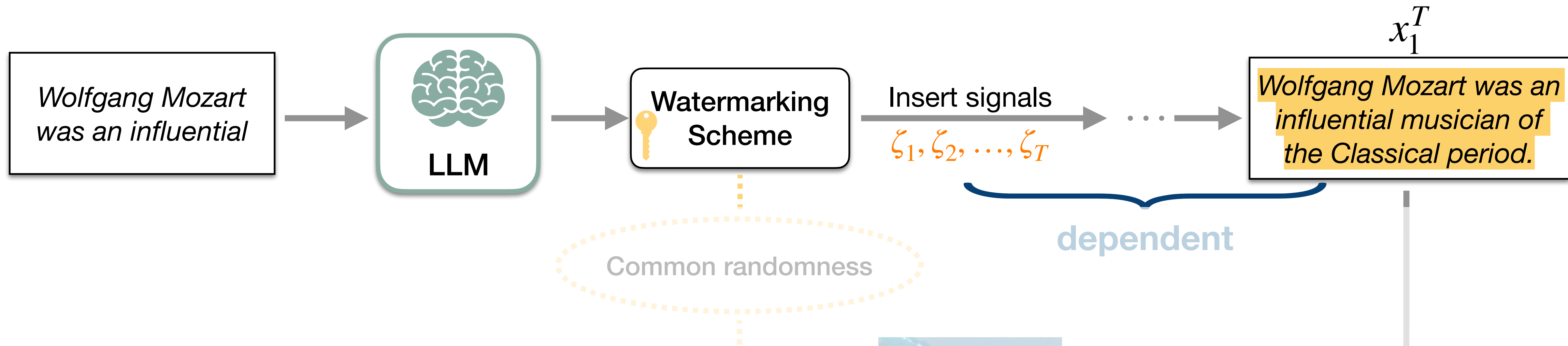
# Hypothesis Testing for LLM Watermark Detection



# Hypothesis Testing for LLM Watermark Detection



# Hypothesis Testing for LLM Watermark Detection



Watermark Detection  $\implies$  Hypothesis Testing:

$$H_0 : X_1^T \text{ is human written, i.e., } (X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$$

$$H_1 : X_1^T \text{ is LLM generated, i.e., } (X_1^T, \zeta_1^T) \sim P_{X_1^T, \zeta_1^T}$$

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing:

$H_0$  :  $X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$$H_0 : X_1^T \text{ is human written, i.e., } (X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$$

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Watermarking scheme

# LLM Watermark Detection Errors

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Watermarking scheme

Performance metric:



# LLM Watermark Detection Errors

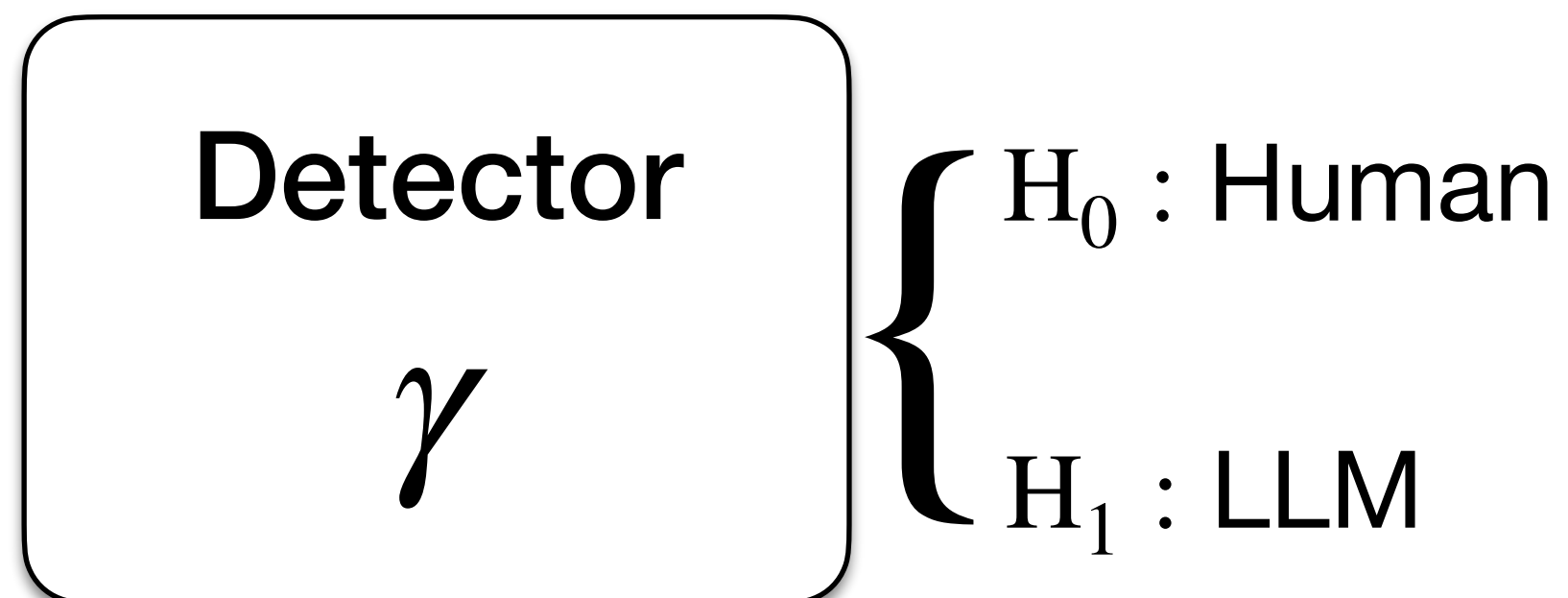
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Watermarking scheme

Performance metric:



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Watermarking scheme

Performance metric:

Reality

$H_0$  : Human

$H_1$  : LLM

Detector

$\gamma$

$\left\{ \begin{array}{l} H_0 : \text{Human} \\ H_1 : \text{LLM} \end{array} \right.$

	$H_0$ : Human	$H_1$ : LLM
Detector $\gamma$		

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$$H_0 : X_1^T \text{ is human written, i.e., } (X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$$

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Watermarking scheme

Performance metric:

Reality

$H_0$  : Human

$H_1$  : LLM

<p>Detector</p> <p><math>\gamma</math></p>	$H_0$ : Human	
	$H_1$ : LLM	<p>Type-I error (false alarm)</p> $\beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T})$

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

Performance metric:

Reality

$H_0$  : Human

$H_1$  : LLM

<p><b>Detector</b></p> <p><math>\gamma</math></p>	$\left\{ \begin{array}{l} H_0 : \text{Human} \\ H_1 : \text{LLM} \end{array} \right.$	<p>✓</p>	<p>Type-II error (miss detection)</p> <p><math>\beta_1(\gamma, P_{X_1^T, \zeta_1^T})</math></p>
		<p>Type-I error (false alarm)</p> <p><math>\beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T})</math></p>	<p>✓</p>

# LLM Watermark Detection Errors

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Watermarking scheme

Performance metric:

Reality

$H_0$  : Human

$H_1$  : LLM

Detector  
 $\gamma$

$\left\{ \begin{array}{l} H_0 : \text{Human} \\ H_1 : \text{LLM} \end{array} \right.$

$\checkmark$	Type-II error (miss detection) $\min \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$
Type-I error (false alarm) $\beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}) \leq \alpha$	$\checkmark$

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$$H_0 : X_1^T \text{ is human written, i.e., } (X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$$

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Watermarking scheme

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Other criteria for LLM watermarking?

scheme

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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Other criteria for LLM watermarking?

$\implies$  **Text Quality!**

scheme



# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

$H_1 : X_1^T$  is LLM generated, i.e.,  $(X_1^T, \zeta_1^T) \sim P_{X_1^T, \zeta_1^T}$

Other criteria for LLM watermarking?

$\implies$  **Text Quality!**

$\implies$  **Indistinguishable from unwatermarked**

scheme

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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Watermarking scheme

watermarked text distribution

$P_{X_1^T}$

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

$H_1 : X_1^T$  is LLM generated, i.e.,  $(X_1^T, \zeta_1^T) \sim P_{X_1^T, \zeta_1^T}$

Watermarking scheme

watermarked text distribution

$P_{X_1^T}$

vs

original text distribution

$Q_{X_1^T}$

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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Watermarking scheme

watermarked text distribution

$P_{X_1^T}$

vs

original text distribution

$Q_{X_1^T}$

Good text quality

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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Watermarking scheme

watermarked text distribution

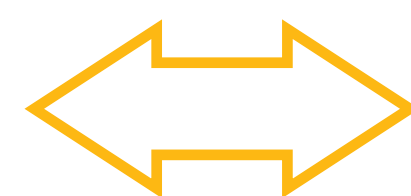
$P_{X_1^T}$

vs

original text distribution

$Q_{X_1^T}$

Good text quality



$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

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Watermarking scheme

watermarked text distribution

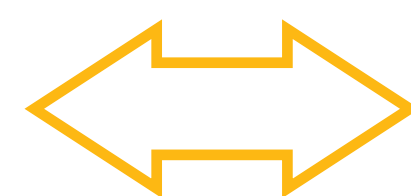
$P_{X_1^T}$

vs

original text distribution

$Q_{X_1^T}$

Good text quality



$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

(Distortion Level)

# LLM Watermarked Text Quality

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$H_0 : X_1^T$  is human written, i.e.,  $(X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$

$H_1 : X_1^T$  is LLM generated, i.e.,  $(X_1^T, \zeta_1^T) \sim P_{X_1^T, \zeta_1^T}$

Watermarking scheme

watermarked text distribution

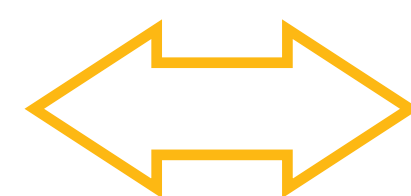
$P_{X_1^T}$

vs

original text distribution

$Q_{X_1^T}$

Good text quality



$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$  (D can be any distortion metric)

(Distortion Level)

# Trade-off in Designing LLM Watermarking

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

$$H_0 : X_1^T \text{ is human written, i.e., } (X_1^T, \zeta_1^T) \sim Q_{X_1^T} \otimes P_{\zeta_1^T}$$

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Watermarking scheme

**Trade-off:**

Type-II error — — False alarm rate — — Distortion Level

$$\beta_1 \text{ — — } \alpha \text{ — — } \epsilon$$

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Existing watermarking methods: **heuristic**

**Example**  
[KGW-1, 2023]

No watermark
Extremely efficient on average term lengths and word frequencies on synthetic, microamount text (as little as 25 words)
Very small and low-resource key/hash (e.g., 140 bits per key is sufficient for 99.999999999% of the Synthetic Internet)

With watermark
- minimal marginal probability for a detection attempt.
- Good speech frequency and energy rate reduction.
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- easy for humans to verify.

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Green word: increase sampling probability

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Existing watermarking methods: **heuristic**

Watermarking scheme

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Very small and low-resource key/hash (e.g., 140 bits per key is sufficient for 99.999999999% of the Synthetic Internet)

With watermark
- minimal marginal probability for a detection attempt.
- Good speech frequency and energy rate reduction.
- messages indiscernible to humans.
- easy for humans to verify.

- High miss detection when requiring low false alarm
- Not distortion-free



# Optimize LLM Watermark Generation and Detection

Watermark Detection  $\implies$  Hypothesis Testing: Human/unwatermarked LLM

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Find the best watermarking scheme & detector:

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Watermarking scheme

Find the best watermarking scheme & detector:

Minimize miss detection

$$\implies \min_{\gamma, P_{X_1^T, \zeta_1^T}} \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$$

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Humans are very creative,  
can write arbitrary texts

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Watermarking scheme

Find the best watermarking scheme & detector:

Humans are very creative,  
can write arbitrary texts

$$\begin{aligned} & \min_{\gamma, P_{X_1^T, \zeta_1^T}} \beta_1(\gamma, P_{X_1^T, \zeta_1^T}) \\ & \text{s.t. } \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}) \leq \alpha \end{aligned}$$

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Ensure text quality  $\rightarrow$

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Ensure text quality

$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$

# Optimize LLM Watermark Generation and Detection

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$$D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon$$



# Fundamental Limit for Type-II Error

## Optimization problem:

$$\min_{\gamma, P_{X_1^T}, P_{\zeta_1^T}} \beta_1(\gamma, P_{X_1^T}, P_{\zeta_1^T})$$

$$\text{s.t. } \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}) \leq \alpha$$

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# Fundamental Limit for Type-II Error

Watermarked text distribution:  $P_{X_1^T}^* = \arg \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{x_1^T} (P_{X_1^T}(x_1^T) - \alpha)_+$

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## ◆ Minimum Type-II error:

$$\beta_1^*(Q_{X_1^T}, \alpha, \epsilon) = \sum_{x_1^T} (P_{X_1^T}^*(x_1^T) - \alpha)_+$$

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**Best achievable for any watermarking methods**

Same as Huang et al. (2023, Theorem 3.2) but under different framework

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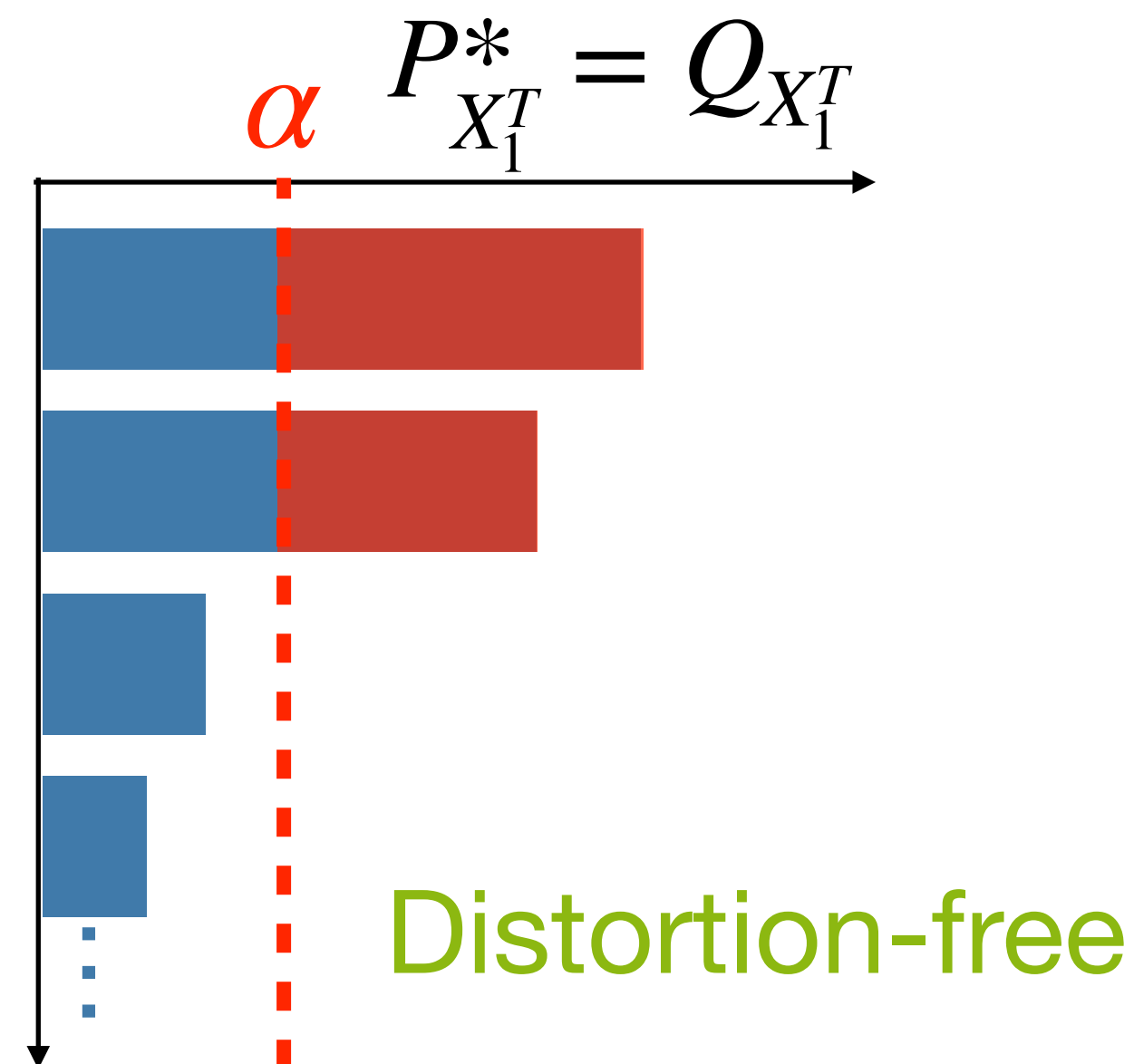
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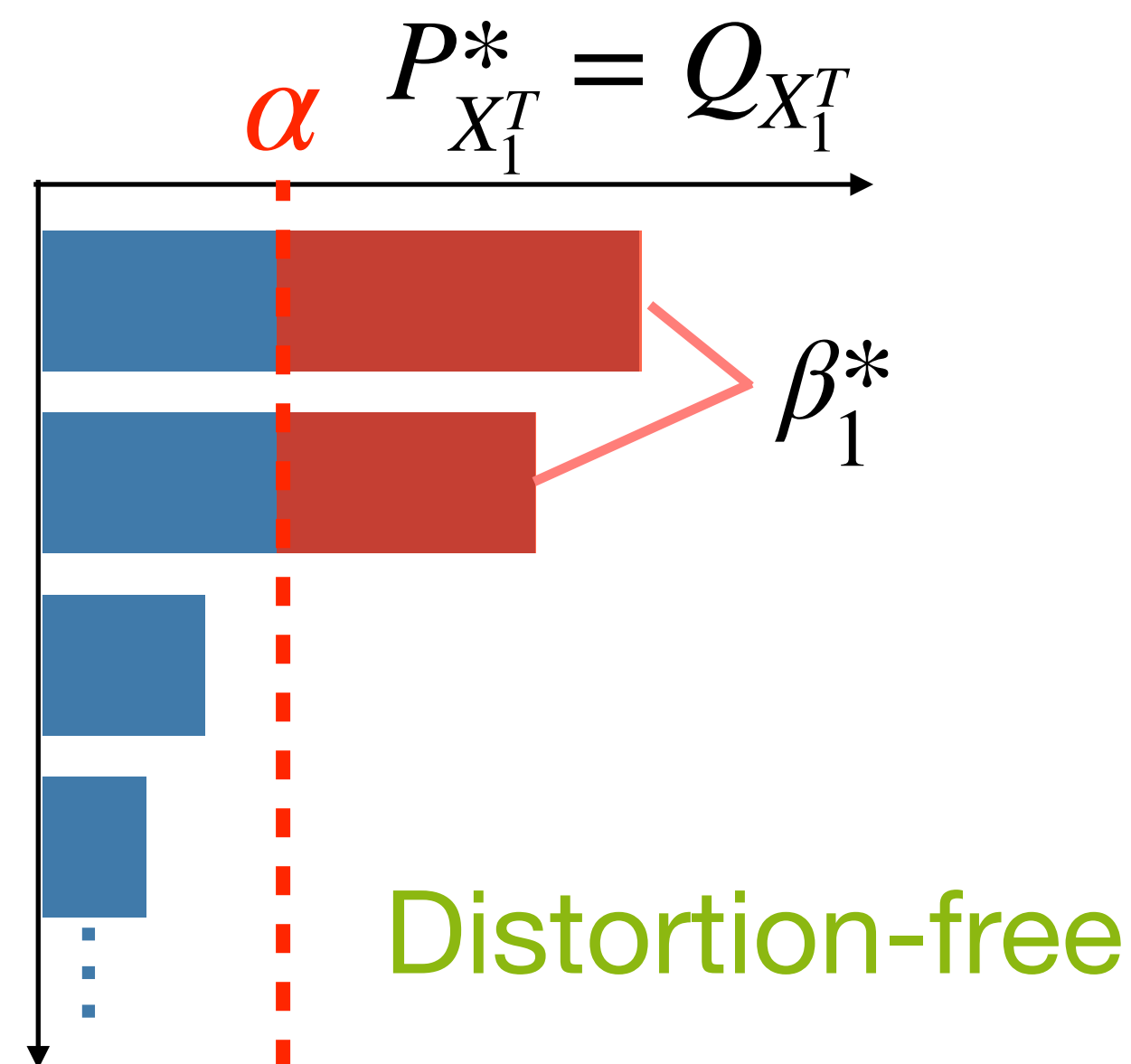
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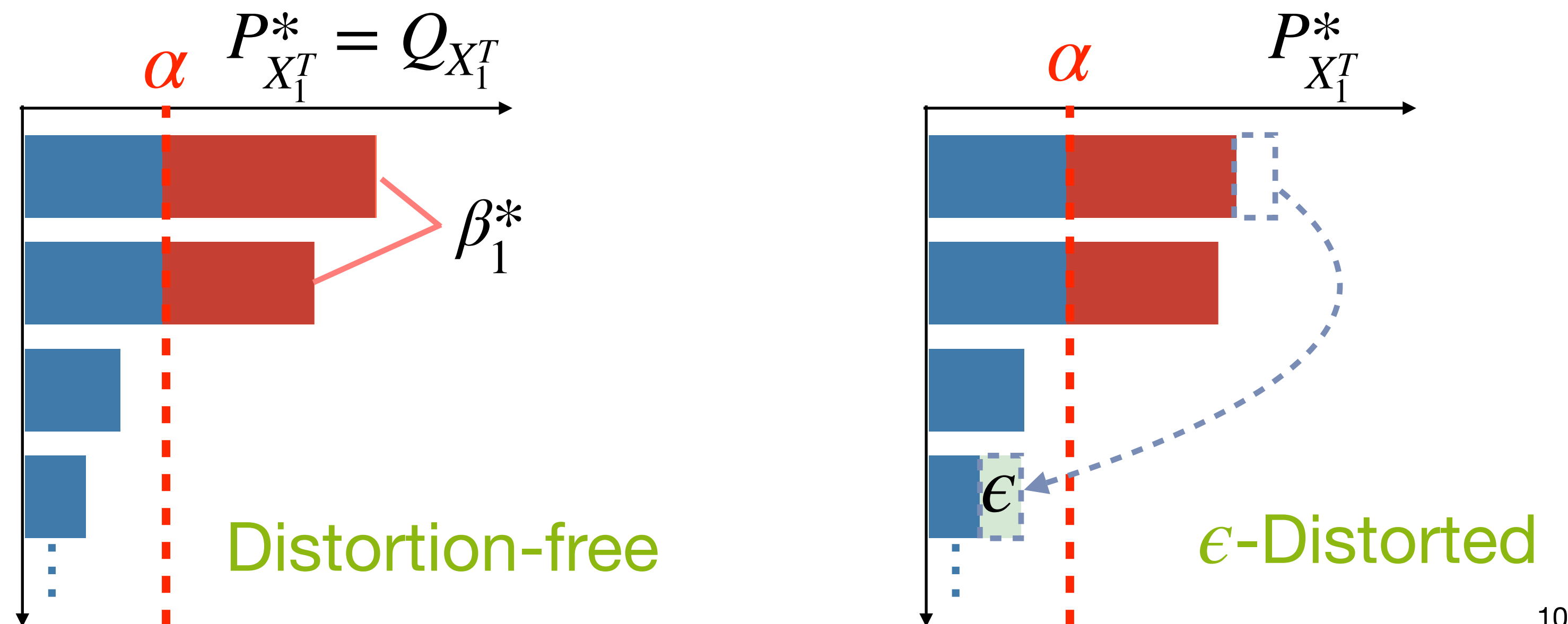
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$D_{TV}$

## ◆ Minimum Type-II error:

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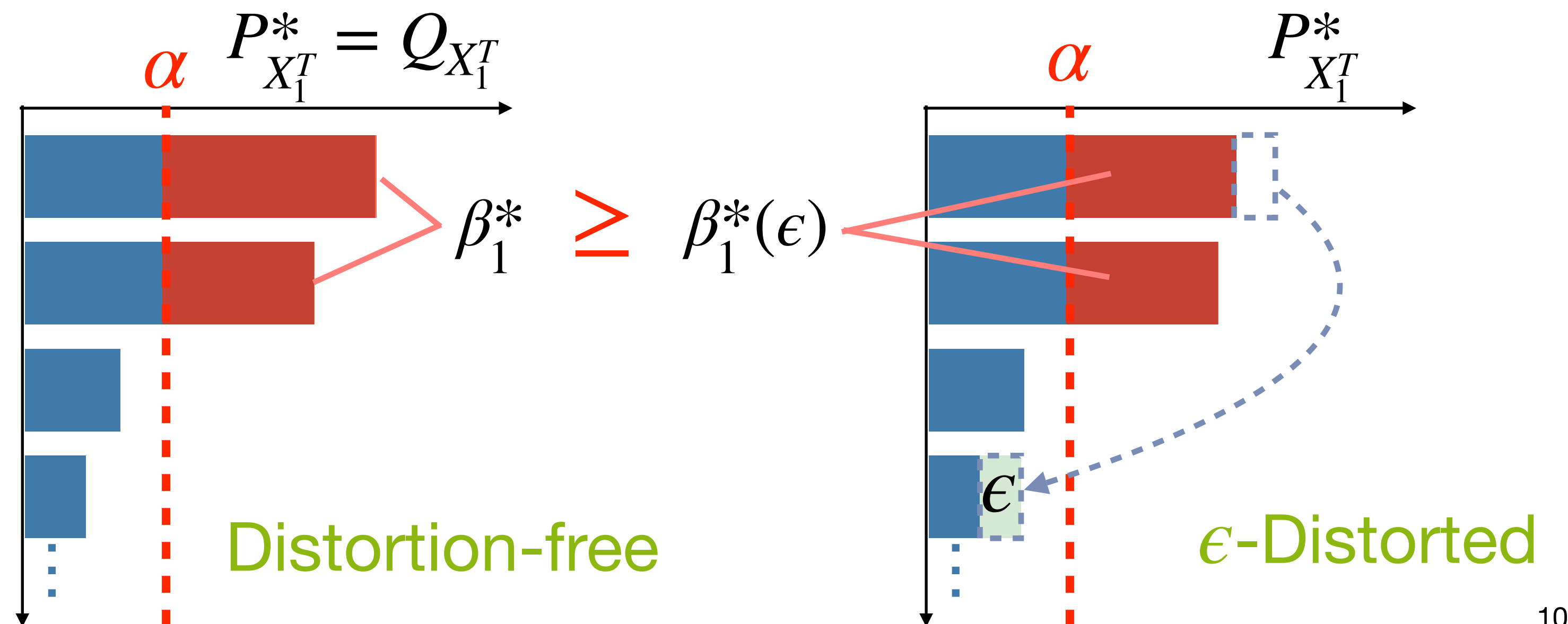
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$D_{TV}$

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# Jointly Optimal Detector and Watermarking Scheme

## Optimization problem:

$$\min_{\gamma, P_{X_1^T, \zeta_1^T}} \beta_1(\gamma, P_{X_1^T, \zeta_1^T})$$

$$\text{s.t. } \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}) \leq \alpha$$

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# Jointly Optimal Detector and Watermarking Scheme

◆ Jointly optimal detector  $\gamma^*$   
and watermarking scheme  $P_{X_1^T, \zeta_1^T}^*$  :

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$$\gamma^* = \mathbf{1}\{X_1^T = g(\zeta_1^T)\}$$

for some surjective  $g : \mathcal{L}^T \rightarrow \mathcal{S} \supset \mathcal{V}^T$

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$$P_{X_1^T, \zeta_1^T}^* :$$

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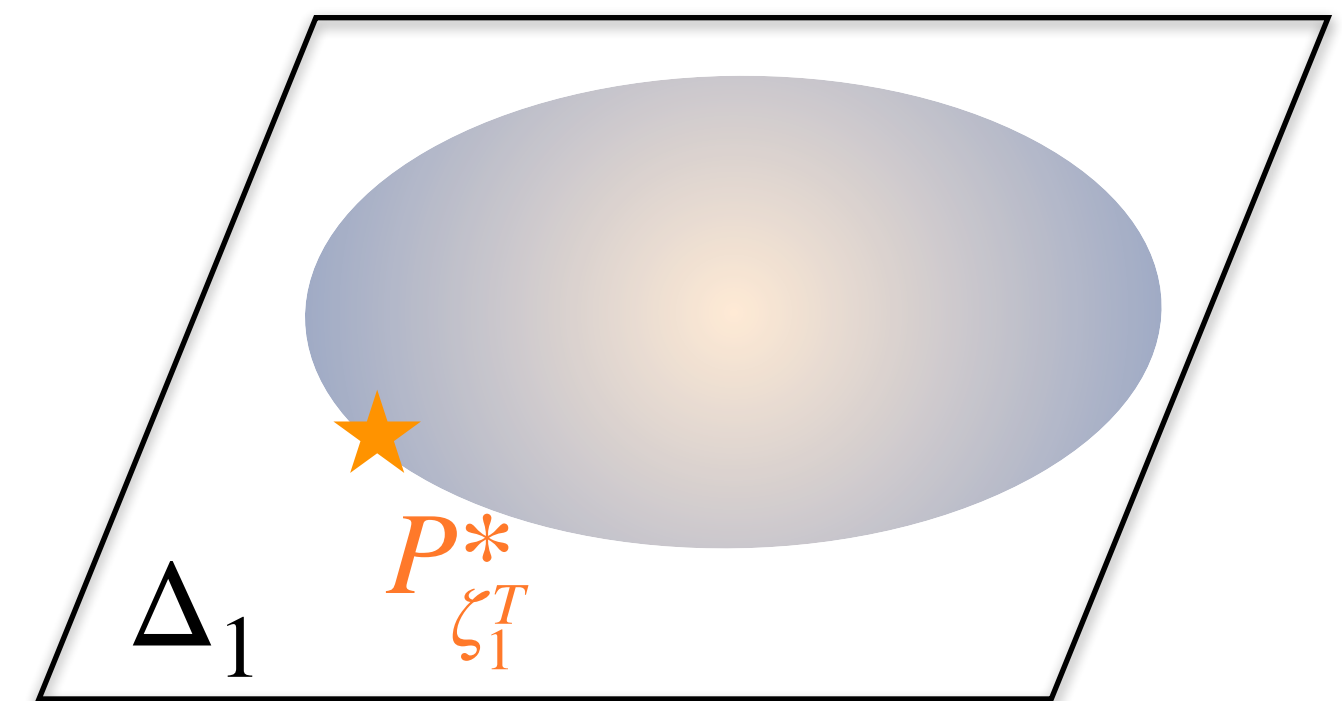
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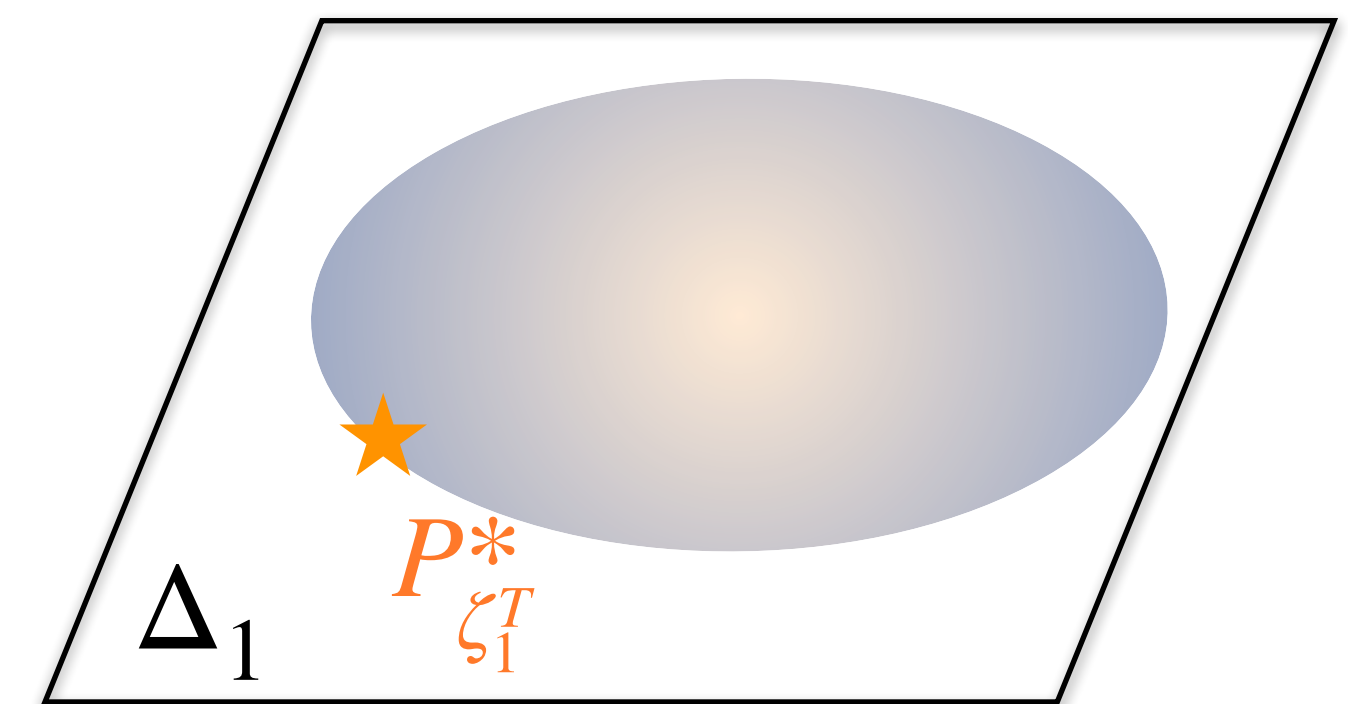
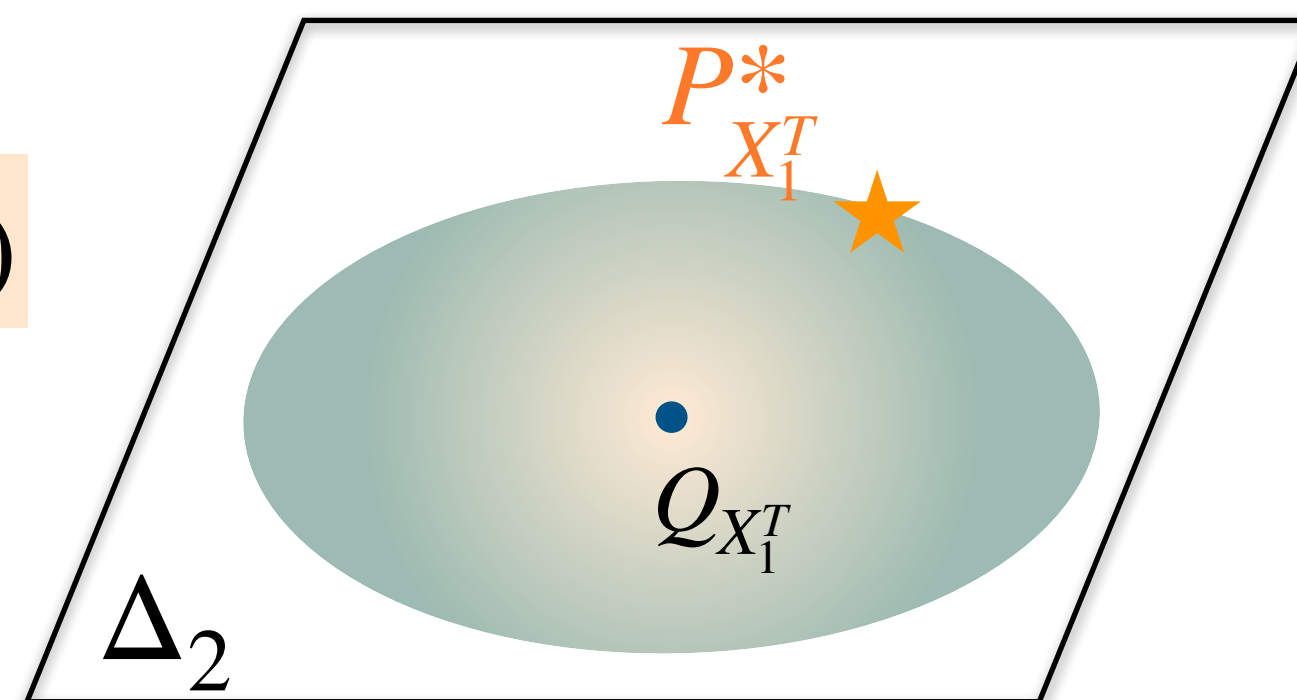
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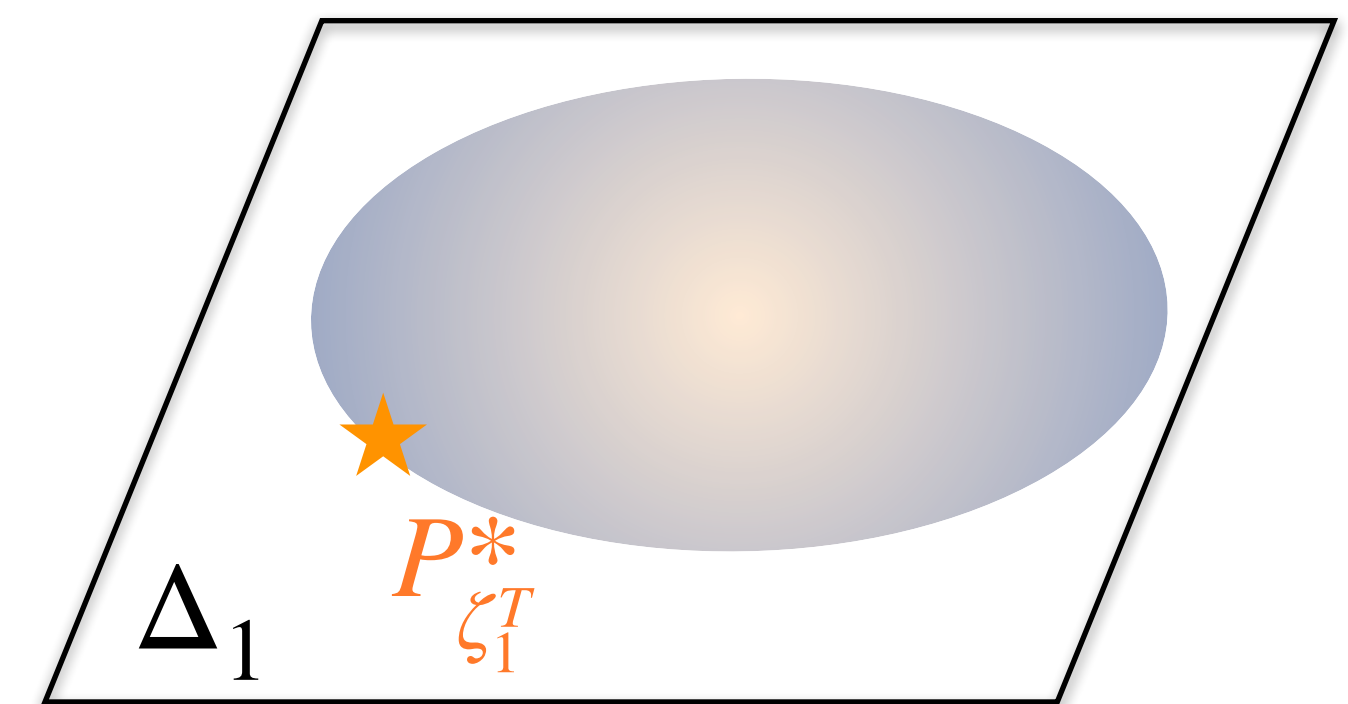
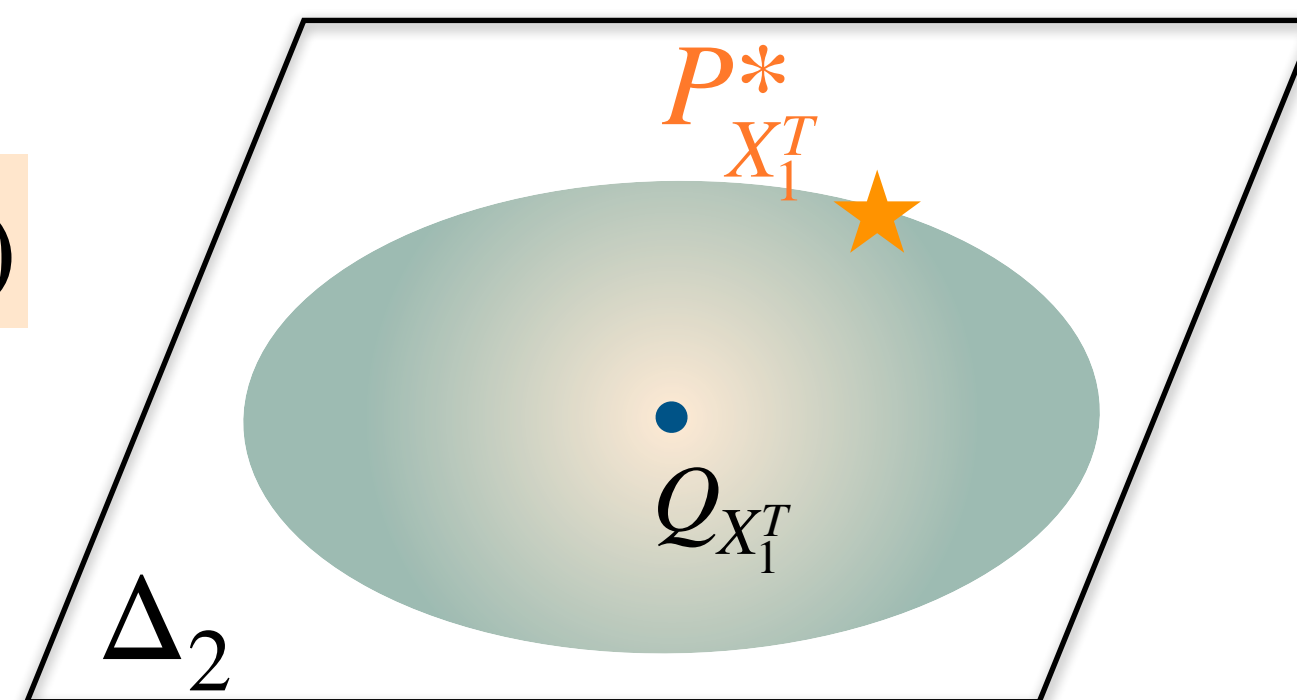
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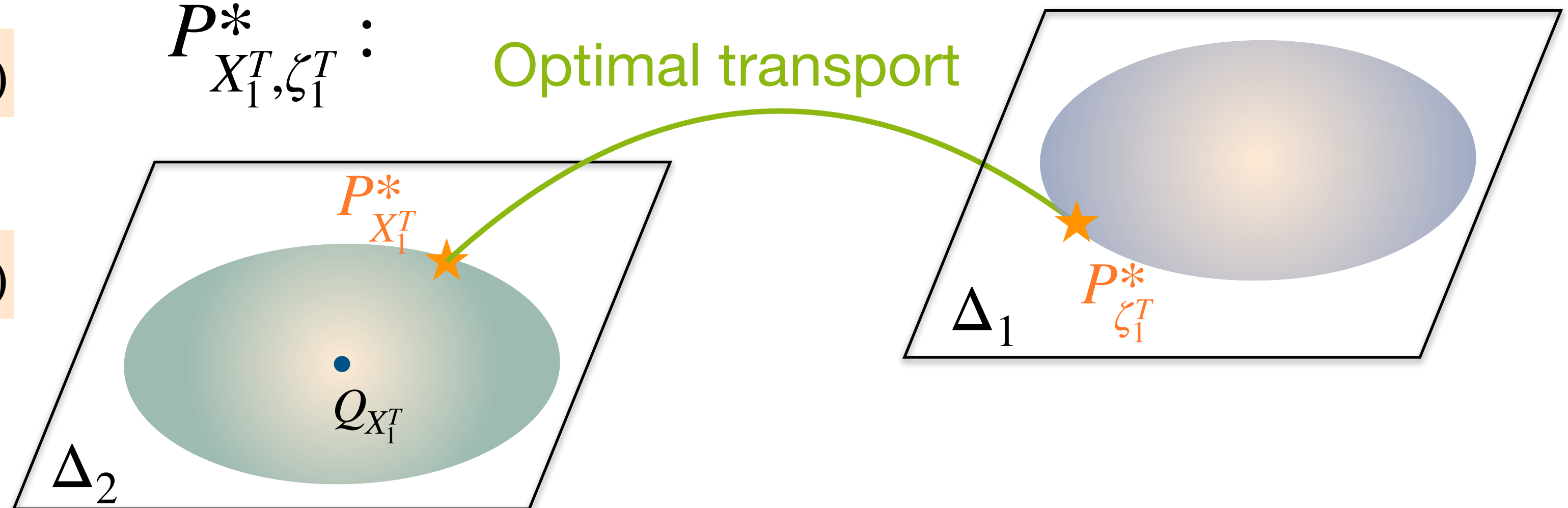
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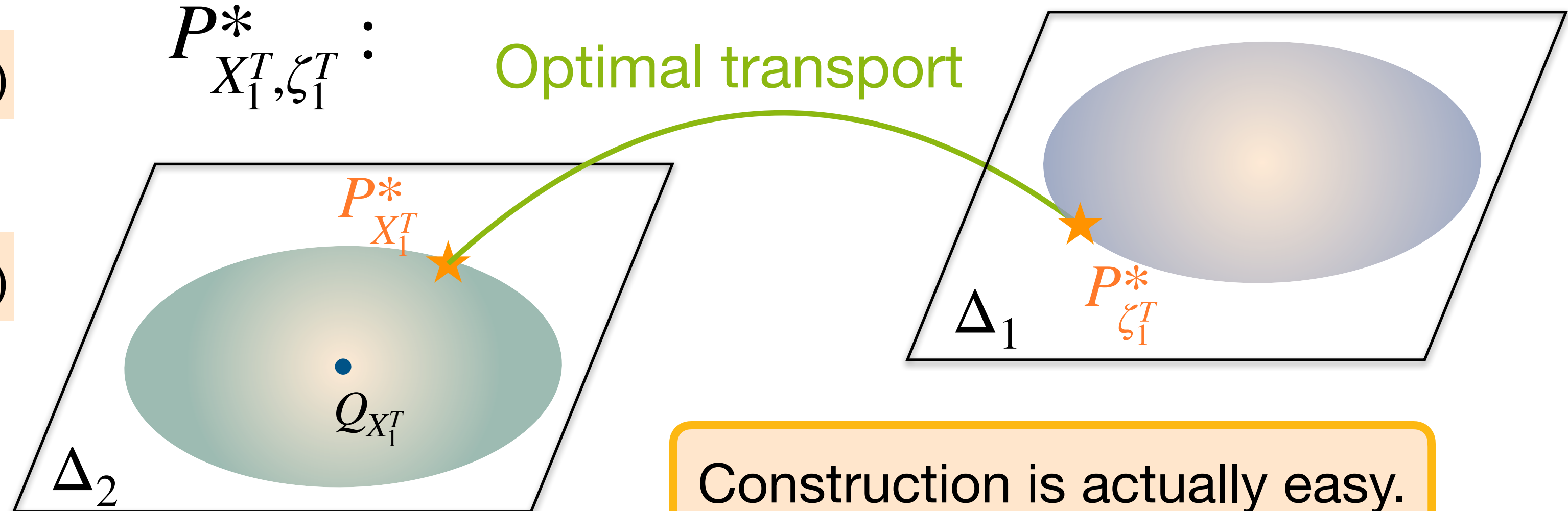
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Construction is actually easy.

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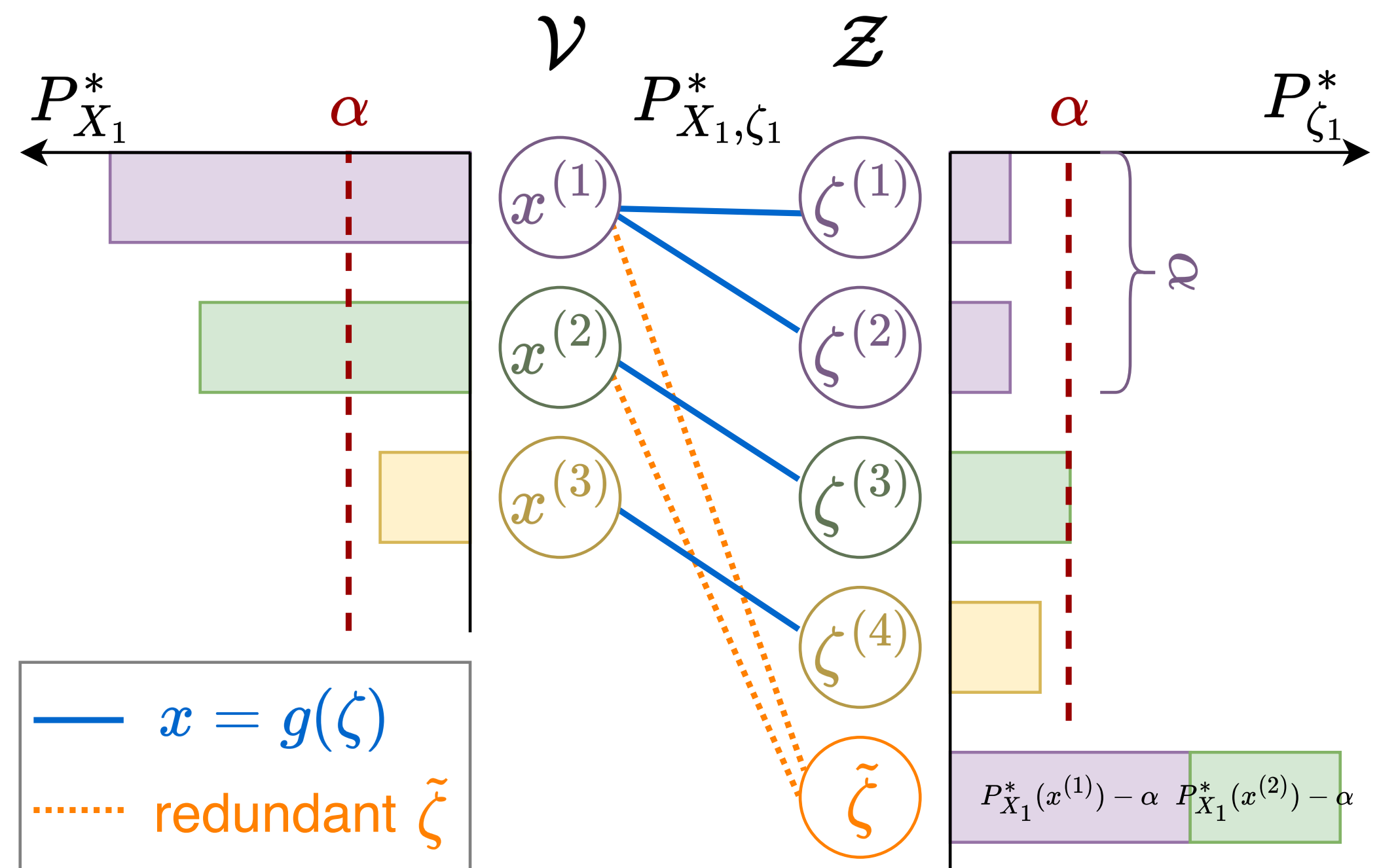
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Unlike existing watermarking methods



# Sequence-Level Optimal to Token-Level Optimal

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$$P_{X_1^T, \zeta_1^T}^* \rightarrow P_{X_t, \zeta_t | X_1^{t-1}, \zeta_1^{t-1}}^*, \forall t = 1, 2, \dots, T$$

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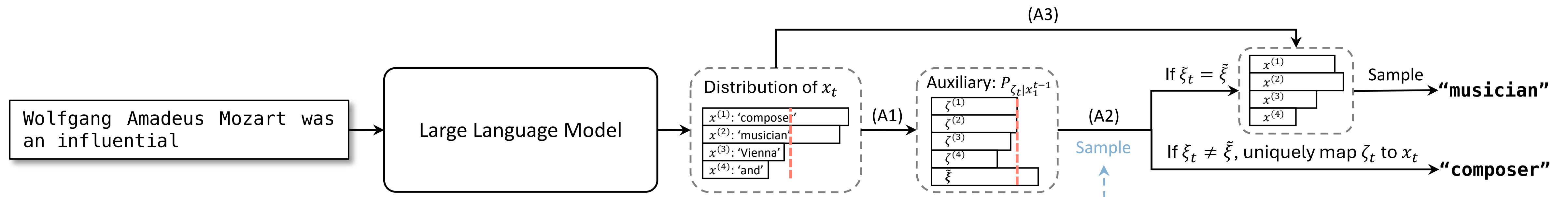
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dependent

Token-level false alarm rate  $\eta$   $\xrightarrow{\text{controls}}$  Sequence-level false alarm  $\alpha$

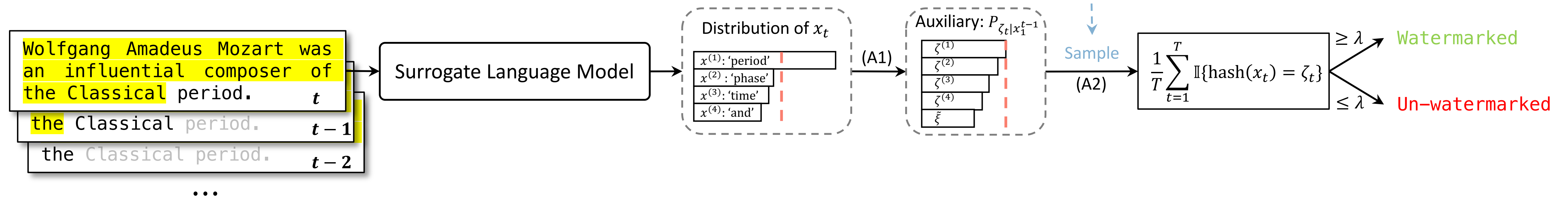
# DAWA: Distribution-Adaptive Watermarking Algorithm

( $\epsilon = 0$ , distortion-free)



Watermark Generation

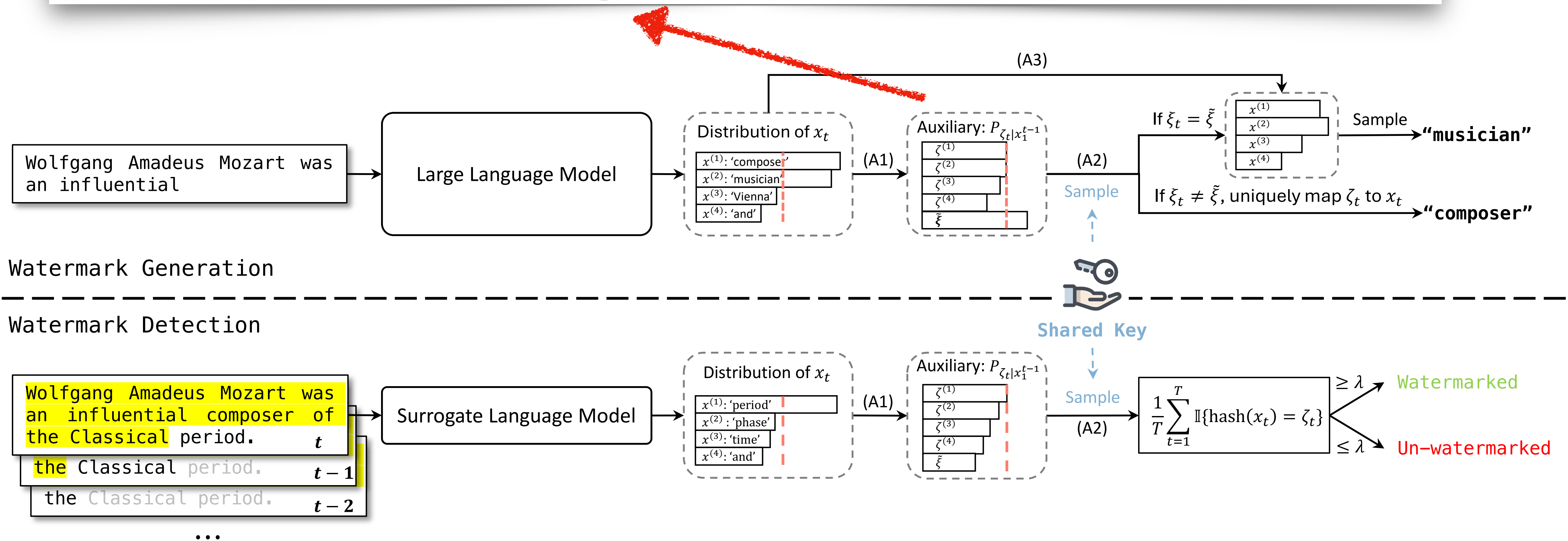
Watermark Detection





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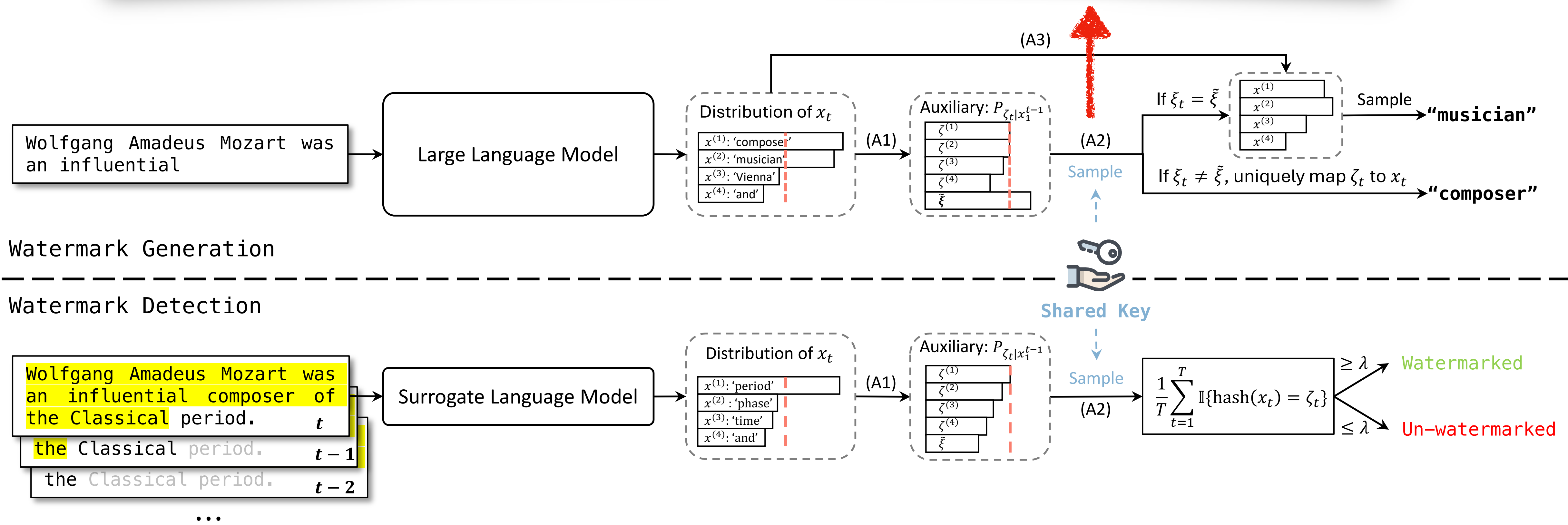
At each time  $t$ , construct  $P_{\zeta_t|X_1^t}^*$  from the LLM predicted distribution  $Q_{X_t|X_1^{t-1}}$



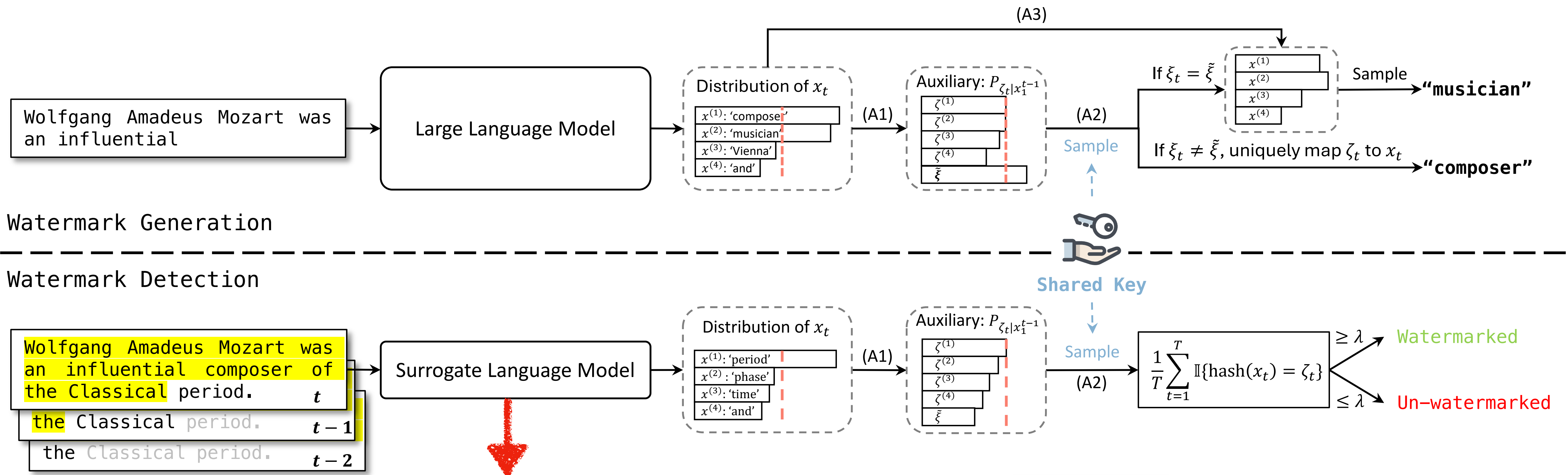
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Sample  $\zeta_t$  using Gumbel max trick:  $\zeta_t \leftarrow \arg \max_{\zeta} \log P_{\zeta_t|x_1^t}^*(\zeta) + G_{\zeta,t}$



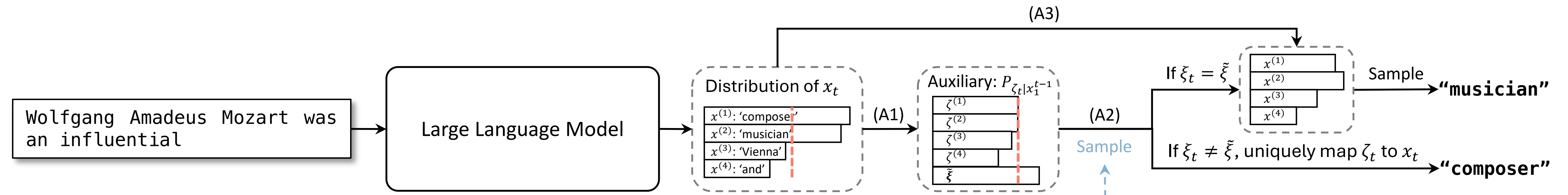
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Approximate distribution of  $X_t$  so as to construct  $\tilde{P}_{\zeta_t|x_1^t}$

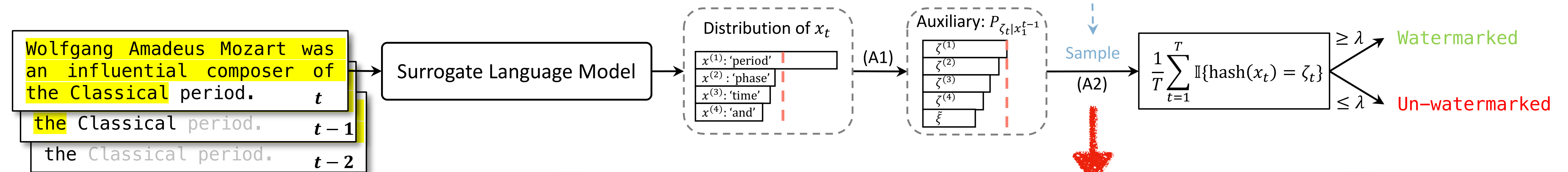
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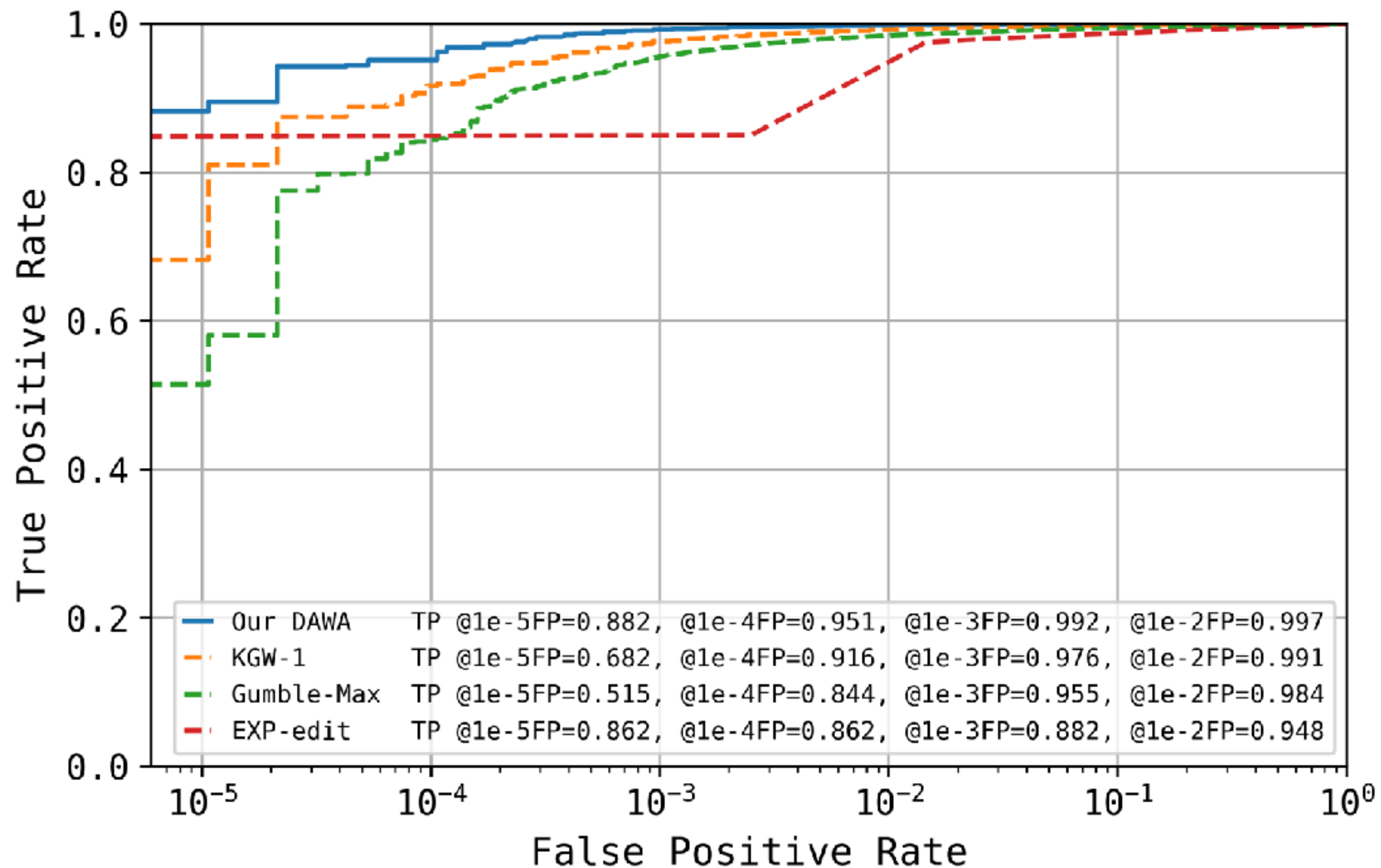
# Experimental Result

**DAWA** (**D**istribution-**A**daptive **W**atermarking **A**lgorithm)

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## DAWA (Distribution-Adaptive Watermarking Algorithm)

Fast and Accurate



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**DAWA** (**D**istribution-**A**daptive **W**atermarking **A**lgorithm)

Fast and  
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Text quality  
high



Methods	Human	KGW-1	EXP-Edit	Gumbel-Max	<b>Ours</b>
BLEU Score	0.219	0.158	0.203	0.210	0.214
Avg Perplexity	8.846	14.327	12.186	11.732	6.495

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# Robustness Against Text Modifications

Optimization problem:

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$$\begin{aligned} \min_{\gamma, P_{X_1^T}, \zeta_1^T} \quad & \beta_1(\gamma, P_{X_1^T}, \zeta_1^T, f) \\ \text{s.t.} \quad & \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}, f) \leq \alpha \\ & D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon \end{aligned}$$

## ◆ Minimum $f$ -robust Type-II error:

$$\begin{aligned} & \beta_1^*(Q_{X_1^T}, \alpha, \epsilon, f) \\ &= \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{k \in [K]} \left( \left( \sum_{x_1^T: f(x_1^T)=k} P_{X_1^T}(x_1^T) \right) - \alpha \right)_+ \end{aligned}$$

Higher than the minimum Type-II error without considering robustness

# Robustness Against Text Modifications

## Optimization problem:

$$\begin{aligned} \min_{\gamma, P_{X_1^T}, \zeta_1^T} \quad & \beta_1(\gamma, P_{X_1^T}, \zeta_1^T, f) \\ \text{s.t.} \quad & \sup_{Q_{X_1^T}} \beta_0(\gamma, Q_{X_1^T}, P_{\zeta_1^T}, f) \leq \alpha \\ & D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon \end{aligned}$$

## ◆ Minimum $f$ -robust Type-II error:

$$\begin{aligned} & \beta_1^*(Q_{X_1^T}, \alpha, \epsilon, f) \\ &= \min_{P_{X_1^T}: D(P_{X_1^T}, Q_{X_1^T}) \leq \epsilon} \sum_{k \in [K]} \left( \left( \sum_{x_1^T: f(x_1^T)=k} P_{X_1^T}(x_1^T) \right) - \alpha \right)_+ \end{aligned}$$

Higher than the minimum Type-II error without considering robustness

## ◆ Optimal watermarking scheme:

add signal  $\zeta_1^T$  to  $P_{f(X_1^T)}$ , e.g., in the semantic space